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REMARKS ON ZAGREB INDICES

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Abstract

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 of the respective graph. We give upper bounds for the Zagreb indices M_1 and M_2 of K_{r+1}-free graphs in terms of the number of vertices and the number of edges, where $r \geq 2$, and determine the graphs for which the bounds are attained. We also consider $K_{1,1,k+1}$- and $K_{2,l+1}$-free graphs, where $0 \leq k \leq l$.

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 recognized in [2] as measures of the branching of the molecular skeleton. These structure–descriptors [3, 4] have been widely used in QSPR and QSAR studies (see [5]). Their main properties were summarized in [6, 7], and some recent results can be found in [8–14].

Let G be a graph with n vertices and m edges. From the definitions of M_1 and M_2, we have

$$M_1(G) = \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} d_v$$

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

For a nonempty subset V_1 of $V(G)$, $G[V_1]$ denotes the subgraph of G induced by V_1. For any $u \in V(G)$, let c_u be the number of edges of the subgraph $G[\Gamma(u)]$ and e_u be the number of edges connecting a vertex in $\Gamma(u)$ and a vertex in $V(G) \setminus (\{u\} \cup \Gamma(u))$. Note that there are d_u edges leading to u. Thus $\sum_{v \in \Gamma(u)} d_v = d_u + 2c_u + e_u$, $e_u \leq m - d_u - c_u$, and then

$$\sum_{v \in \Gamma(u)} d_v \leq m + c_u \tag{1}$$

with equality for $d_u > 0$ if and only if either $d_u = n - 1$ or $G[V(G) \setminus (\{u\} \cup \Gamma(u))]$ is an empty graph if $d_u < n - 1$.

We now give upper bounds for the Zagreb indices M_1 and M_2 of K_{r+1}-free graphs in terms of the number of vertices and the number of edges, where $r \geq 2$, and determine the graphs for which the bounds are attained. We also consider $K_{1,1,k+1}$- and $K_{2,l+1}$-free graphs, where $0 \leq k \leq l$.

UPPER BOUNDS FOR M_1 AND M_2

Let G be a K_{r+1}-free graph with n vertices, where $r \geq 2$. If $r \geq n$, then obviously $M_1(G) \leq M_1(K_n)$ and $M_2(G) \leq M_2(K_n)$ with either equality if and only if $G \cong K_n$. So in the following we suppose that $2 \leq r \leq n - 1$.

Theorem 1. *Let G be a K_{r+1}-free graph with n vertices and $m > 0$ edges, where $2 \leq r \leq n - 1$. Then*

$$M_1(G) \leq \frac{2r-2}{r} nm \tag{2}$$

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

with either equality if and only if G is a complete bipartite graph for $r = 2$ and a regular complete r-partite graph for $r \geq 3$.

Proof. Let u be any vertex of G. The subgraph $G[\Gamma(u)]$ may not contain a K_r as a subgraph and thus, by Turán's theorem (see [15]), $c_u \leq \frac{r-2}{2r-2}\,(d_u)^2$ with equality if and only if $G[\Gamma(u)]$ is a regular complete $(r-1)$-partite graph (where a complete 1-partite graph is an empty graph). From (1),

$$\sum_{v \in \Gamma(u)} d_v \leq m + \frac{r-2}{2r-2}\,(d_u)^2$$

and thus

$$M_1(G) \leq \sum_{u \in V(G)} \left[m + \frac{r-2}{2r-2}\,(d_u)^2 \right] = nm + \frac{r-2}{2r-2}\,M_1(G)$$

from which we have (2).

Note that

$$\begin{aligned}
\sum_{u \in V(G)} (d_u)^3 &= \tfrac{1}{2} \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} [(d_u)^2 + (d_v)^2] \\
&= \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} d_u d_v + \tfrac{1}{2} \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} (d_u - d_v)^2 \\
&= 2M_2(G) + \tfrac{1}{2} \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} (d_u - d_v)^2 \\
&\leq 2M_2(G) + \tfrac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} (d_u - d_v)^2 \\
&= 2M_2(G) + \tfrac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} [(d_u)^2 + (d_v)^2] - \sum_{u \in V(G)} \sum_{v \in V(G)} d_u d_v \\
&= 2M_2(G) + nM_1(G) - 4m^2.
\end{aligned}$$

It is easy to see that

$$\begin{aligned}
M_2(G) &\leq \tfrac{1}{2} \sum_{u \in V(G)} d_u \left[m + \tfrac{r-2}{2r-2}\,(d_u)^2 \right] = m^2 + \tfrac{r-2}{4r-4} \sum_{u \in V(G)} (d_u)^3 \\
&\leq m^2 + \tfrac{r-2}{4r-4}\,[2M_2(G) + nM_1(G) - 4m^2]
\end{aligned}$$

and then

$$M_2(G) \leq \frac{2}{r}\,m^2 + \frac{r-2}{2r}\,nM_1(G)$$

which, together with (2), implies (3).

Suppose that equality holds in (2). Then equality holds in (1) and $c_u = \frac{r-2}{2r-2}\,(d_u)^2$ for any $u \in V(G)$. Thus for any $u \in V(G)$, $G[\Gamma(u)]$ is a regular complete $(r-1)$-partite graph, and $d_u = n-1$ or $G[V(G) \setminus (\{u\} \cup \Gamma(u))]$ is an empty graph if $d_u < n-1$. Let v and w be any pair of distinct vertices that are not adjacent. Suppose that there is a vertex $z \in \Gamma(v) \setminus \Gamma(w)$. Then $vz \in E(G)$, and $v, z \in V(G) \setminus (\{w\} \cup \Gamma(w))$. Thus $d_w < n-1$, but $G[V(G) \setminus (\{w\} \cup \Gamma(w))]$ is not an empty graph, which is a contradiction. So $\Gamma(v) \subseteq \Gamma(w)$ and then $\Gamma(v) = \Gamma(w)$. Thus $G \cong K_{n-d_u, \frac{d_u}{r-1}, \ldots, \frac{d_u}{r-1}}$ for any $u \in V(G)$. Now it is easy to see that G is a complete bipartite graph if $r = 2$ and $G \cong K_{\frac{n}{r}, \ldots, \frac{n}{r}}$ if $r \geq 3$.

Suppose that equality holds in (3). Then equality holds in (1) and $c_u = \frac{r-2}{2r-2}(d_u)^2$ for any $u \in V(G)$. So G is a complete bipartite graph for $r = 2$ and a regular complete $(r-1)$-partite graph for $r \geq 3$.

Conversely, it is easy to check that (2) and (3) are both equalities if G is a complete bipartite graph for $r = 2$ or a regular complete $(r-1)$-partite graph for $r \geq 3$. $\square$

Remark 2. The case of K_3-free graphs has been treated in [10]. Let G be a K_4-free graph with $n \geq 3$ vertices and $m > 0$ edges. From [14], we have

$$M_1(G) \leq \frac{4nm - 2s}{3}$$

with equality if and only if $G \cong K_{\lfloor \frac{n}{3} \rfloor, \lfloor \frac{n+1}{3} \rfloor, \lfloor \frac{n+2}{3} \rfloor}$, where $2s$ is the number of vertices of odd degrees in G.

Remark 3. Let G be a $K_{1,1,k+1}$- and $K_{2,l+1}$-free graph with n vertices and $m > 0$ edges, where $0 \leq k \leq l$. The cases $k = l$ (i.e., $K_{2,l+1}$-free graph) and $k = 0$, $l = 1$ (i.e., triangle- and quadrangle-free graph) have been treated in [13]. Since G is $K_{1,1,k+1}$-free, a vertex from $\Gamma(u)$ has at most k neighbors in $\Gamma(u)$, and so $2c_u \leq kd_u$. Since G is $K_{2,l+1}$-free, a vertex from $V(G) \setminus (\{u\} \cup \Gamma(u))$ has at most l neighbors in $\Gamma(u)$, and so $e_u \leq l(n - d_u - 1)$. It follows that

$$\sum_{v \in \Gamma(u)} d_v = d_u + 2c_u + e_u \leq d_u + kd_u + l(n - d_u - 1) = (k + 1 - l)d_u + l(n-1).$$

Now we can easily prove that

$$M_1(G) \leq 2(k + 1 - l)m + ln(n-1)$$

$$M_2(G) \leq (k + 1 - l)^2 m + l(n-1)m + \frac{1}{2}(k + 1 - l)ln(n-1)$$

with either equality if and only each pair of adjacent vertices in G has exactly k common neighbors and each pair of non-adjacent vertices in G has exactly l common neighbors.

Remark 4. Let G be a graph with n vertices, m edges and minimum vertex degree $\delta \geq 1$. Note that for all $u \in V(G)$,

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

with equality if and only if either $d_u = n-1$ or all vertices not adjacent to u are of degree δ. Thus

$$M_2(G) \leq \frac{1}{2} \sum_{u \in V(G)} d_u[2m - d_u - (n-1-d_u)\delta] = 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)M_1(G)\,.$$

We can find upper bounds for $M_2(G)$ depending on n, m and δ by using the upper bounds for $M_1(G)$ (see [13, 14]).

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