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FURTHER PROPERTIES OF 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 underlying molecular graph. We present upper bounds for M_1 and M_2 in terms of the number of vertices, number of edges, minimum vertex degree and maximum vertex degree.

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:

$$M_1 = M_1(G) = \sum_{\text{vertices}} (d_u)^2 \tag{1}$$

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

where d_u stands for the degree of the 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, 4]. Some recent results on the Zagreb indices are reported in [5–8], where also references to the previous mathematical research in this area can be found. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure–descriptors [9, 10].

In this article, we present upper bounds for M_1 and M_2 in terms of the number of vertices (n), the number of edges (m), minimum vertex degree (δ) and maximum vertex degree (Δ).

In what follows it will be required that $\delta \geq 1$ and that $\delta < \Delta$. The former relation is satisfied by all connected graph. Recall that molecular graphs are necessarily connected. The latter relation is satisfied by all non-regular graphs. The majority of graphs of interest in chemical graph theory are non-regular. Note, however, that the molecular graph of ethane/ethylene is regular of degree 1, the molecular graphs of annulenes are regular of degree 2, whereas the molecular graphs of fullerenes are regular of degree 3. For these molecular graphs the bounds deduced in the present paper are not applicable. For all other molecular graphs these bounds are applicable.

UPPER BOUNDS FOR M_1

In [8], within a study of the variance of vertex degrees, an upper bound for M_1 was established, in terms of n, m, and Δ. Employing a similar proof technique as in [8], we now provide a further upper bound for M_1.

Theorem 1. *Let G be a graph with n vertices, m edges, minimum vertex degree $\delta \geq 1$, and maximum vertex degree $\Delta > \delta$. Then*

$$M_1(G) \leq 2m\,(\delta + \Delta) - n\,\delta\,\Delta + (\delta - k)(\Delta - k) \tag{2}$$

where k is the integer defined via

$$2m - n\,\delta \equiv k - \delta \pmod{(\Delta - \delta)} \quad , \quad \delta \leq k \leq \Delta - 1 \tag{3}$$

i. e.,

$$k = 2m - \delta\,(n-1) - (\Delta - \delta) \left\lfloor \frac{2m - n\,\delta}{\Delta - \delta} \right\rfloor .$$

Equality in (2) is attained if and only if at most one vertex of G has degree different from δ and Δ.

Proof. Let n_i be the number of vertices of degree i in the graph G, $\delta \leq i \leq \Delta$. Then Eq. (1) can be rewritten as

$$M_1(G) = \sum_{i=\delta}^{\Delta} i^2\, n_i \ . \tag{4}$$

In addition to this,

$$\sum_{i=\delta}^{\Delta} n_i \;=\; n \tag{5}$$

$$\sum_{i=\delta}^{\Delta} i\, n_i \;=\; 2m \ . \tag{6}$$

By solving (5) and (6) in the variables n_δ and n_Δ we obtain

$$n_\delta \;=\; \frac{1}{\Delta-\delta}\left[n\,\Delta - 2m + \sum_{i=\delta+1}^{\Delta-1}(i-\Delta)\, n_i\right] \tag{7}$$

$$n_\Delta \;=\; \frac{1}{\Delta-\delta}\left[2m - n\,\delta + \sum_{i=\delta+1}^{\Delta-1}(\delta-i)\, n_i\right] \ . \tag{8}$$

By substituting Eqs. (7) and (8) back into (4) we arrive at

$$\begin{aligned} M_1(G) \;&=\; \frac{1}{\Delta-\delta}\left[\delta^2\,(n\,\Delta-2m)+\Delta^2\,(2m-n\,\delta)\right] \\ &+\; \frac{1}{\Delta-\delta}\sum_{i=\delta+1}^{\Delta-1}\left[\delta^2\,(i-\Delta)+\Delta^2\,(\delta-i)+i^2\,(\Delta-\delta)\right]\, n_i \end{aligned}$$

from which it follows

$$M_1(G) = 2m + (\delta+\Delta) - n\,\delta\,\Delta + \sum_{i=\delta+1}^{\Delta-1}(\delta-i)(\Delta-i)\, n_i \ . \tag{9}$$

Observe that the term $(\delta-i)(\Delta-i)$ is strictly negative for $\delta+1 \leq i \leq \Delta-1$. Therefore, for fixed values of n, m, δ, and Δ, the first Zagreb index of a graph G will be maximum if $n_i = 0$ for $i = \delta+1, \ldots, \Delta-1$, provided such a choice of the parameters is possible. In this case, (7) and (8) lead to

$$n_\delta \;=\; \frac{n\,\Delta-2m}{\Delta-\delta}$$

$$n_\Delta \;=\; \frac{2m-n\,\delta}{\Delta-\delta} \ .$$

The above formulas require that

$$2m - n\,\delta \equiv 0 \pmod{(\Delta-\delta)} \tag{10}$$

since n_δ and n_Δ must be integers, and $n\,\Delta - 2m = n\,\delta - 2m + n\,(\Delta - \delta)$.

Suppose now that the condition (10) is not satisfied. If so, then let k be the integer defined via relation (3). It is always possible to choose n_i such that $n_k = 1$ and $n_i = 0$ for all $i = \delta+1, \ldots, \Delta-1$, except for $i = k$. Then Eqs. (7) and (8) become

$$n_\delta = \frac{n\,\Delta - 2m + k - \Delta}{\Delta - \delta}$$

$$n_\Delta = \frac{2m - (n-1)\,\delta - k}{\Delta - \delta}$$

which have integer values and which satisfy the conditions (5) and (6). There always exists a graph with n vertices and all degrees equal to δ (except one vertex with degree 0 if n and δ are both odd) [11]. By adding edges to this graph we may increase the vertex degrees one at a time up to Δ, as long as this is possible. Since $2m - n\,\delta \equiv k - \delta \pmod{(\Delta - \delta)}$, the degree of one more vertex can be increased, up to k. Consequently, there exists a graph with n vertices and m edges, possessing a unique vertex of degree different from δ and Δ, whose degree is equal to k.

Assume now that in the graph G there are two vertices, of degree i and j, such that $\delta+1 \le i \le j \le \Delta-1$. Reducing the degree of the first vertex by 1 and increasing the degree of the second vertex by 1 leaves the sum of vertex degrees unchanged, whereas – in view of Eq. (9) – the value of the first Zagreb index is changed by

$$\begin{aligned} [\delta - (i-1)][\Delta - (i-1)] - (\delta - i)(\Delta - i) & + \\ [\delta - (j+1)]\,[\Delta - (j+1)] - (\delta - j)(\Delta - j) & = 2(j - i + 1) > 0\,. \end{aligned}$$

This means that if the condition (10) is not obeyed, then the optimal choice for the quantities n_i is $n_i = 0$ for all i, $\delta+1 \le i \le \Delta-1$, except for $i = k$, for which $n_k = 1$. If so, then by (9),

$$M_1(G) \le 2m\,(\delta + \Delta) - n\,\delta\,\Delta - (\delta - k)(\Delta - k)\,. \tag{11}$$

Observe that if condition (10) is satisfied, then (3) gives $k = \delta$, which is tantamount to the fact that for $\delta + 1 \le i \le \Delta - 1$, all n_i are equal to zero. Consequently, relation (11) remains valid.

Form the above arguments, it immediately follows that the equality in (2) holds if and only if at most one vertex of G has degree different from δ and Δ. □

It is easy to see that

$$2m\,(\delta + \Delta) - n\,\delta\,\Delta + (\delta - k)(\Delta - k) \le 2m\,(1 + \Delta) - n\,\Delta + (1 - k)(\Delta - k)$$

with equality if and only if $\delta = 1$. Therefore, by setting $\delta = 1$ in the statement of Theorem 1 we arrive at the upper bound previously reported in [8]:

Corollary 2. *Let G be a connected graph with n vertices, m edges and maximum vertex degree $\Delta \geq 3$. Then*

$$M_1(G) \leq 2m\,(1+\Delta) - n\,\Delta + (1-k)(\Delta - k) \tag{12}$$

where k is the integer defined via

$$2m - n \equiv k - 1 \ (mod\ (\Delta - 1)),\ 1 \leq k \leq \Delta - 1$$

i. e.,

$$k = 2m - n + 1 - (\Delta - 1)\left\lfloor \frac{2m-n}{\Delta - 1} \right\rfloor .$$

Equality in (12) is attained if and only if at most one vertex of G has degree different from 1 and Δ.

From Corollary 2 we immediately obtain:

Corollary 3. *Let G be a chemical graph with $n \geq 2$ vertices and m edges. Then*

$$M_1(G) \leq \begin{cases} 10m - 4n & \text{if } 2m - n \equiv 0 \ (mod\ 3)\ , \\ 10m - 4n - 2 & \text{otherwise} \end{cases}$$

with equality if and only if either (i) every vertex of G is of degree 1 or 4 (in which case it must be $2m - n \equiv 0 \ (mod\ 3)$), or (ii) one vertex of G has degree 2 or 3, and all other vertices are of degree 1 or 4.

Recall that in the hydrogen–filled molecular graphs of saturated hydrocarbons (sometimes referred to as *plerograms*) [12] all vertices have degrees 1 or 4.

AN UPPER BOUND FOR M_2

We deduce now an upper bound for M_2 by using the bound for M_1 from Theorem 1.

Theorem 4. *Let G be a graph with n vertices, m edges, minimum vertex degree $\delta \geq 1$, and maximum vertex degree $\Delta > \delta$. Then*

$$M_2(G) \leq 2\,m^2 - (n-1)\,m\,\delta + \frac{1}{2}\,(\delta - 1)\,[2m\,(\delta + \Delta) - n\,\delta\,\Delta + (\delta - k)(\Delta - k)]$$

where k is the integer defined by relation (3).

Proof. Let E stand for the edge set of G, and let $N(v_i)$ be the neighborhood of vertex v_i of G. Note that [5]

$$\begin{aligned} M_2(G) &= \sum_{v_i v_j \in E} d_{v_i} d_{v_j} \\ &= \frac{1}{2} \sum_{i=1}^{n} d_{v_i} \sum_{v_j \in N(v_i)} d_{v_j} \\ &\leq \frac{1}{2} \sum_{i=1}^{n} d_{v_i} \left[2m - d_i - (n-1-d_{v_i})\, \delta\right] \\ &= 2m^2 - (n-1)\, m\, \delta + \frac{1}{2} (\delta - 1)\, M_1(G) \, . \end{aligned}$$

Theorem 4 follows now from Theorem 1. □

Clearly, the upper bound in Theorem 4 can be attained if and only if for every vertex v_i either $d_{v_i} = n-1$ or all the vertices v_j not adjacent to v_i are of degree δ, and at most one vertex of G has degree different from δ and Δ.

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