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SOME PROPERTIES OF THE SECOND ZAGREB INDEX

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Abstract

The graph invariant M_2, known under the name *second Zagreb index*, equal to the sum of the products of the degrees of pairs of adjacent vertices of the respective (molecular) graph, was first considered in 1972. Since then, almost no result for M_2 was communicated in either the chemical or in mathematical literature. In this paper we state and prove a number of results for M_2 — identities and inequalities, including relations between the M_2-index of a graph and its complement.

INTRODUCTION

Long time ago [1], within the study of the dependence of total π-electron energy on molecular structure, some expressions were deduced, containing terms of the form.

$$M_1 = \sum_{\text{vertices}} (d_i)^2 \quad ; \quad M_2 = \sum_{\text{edges}} d_i \cdot d_j$$

with d_i standing for the degree (number of first neighbors) of the vertex v_i of the molecular graph. These terms are, in fact, measures of branching of the molecular carbon-atom skeleton [2] and can thus be viewed as molecular structure-descriptors [3, 4]. In the chemical literature, M_1 and M_2 are called the *first Zagreb-Group index* and the *second Zagreb-Group index*, respectively, or — shorter — the *first Zagreb index* and *second Zagreb index* [3, 4]. For more details on this matter see the recent review [5].

Independently of its chemical context, the sum of squares of vertex degrees of a graph (which, of course, is just the first Zagreb index) was studied by quite a few mathematicians; for details and references see [6]. As a consequence, numerous results on M_1 are nowadays known [6, 7, 8].

The second Zagreb index attracted so far almost no attention of mathematicians and/or mathematical chemists and — to our best knowledge — not a single general property of M_2 was reported in the literature. This motivated us to try to establish a few such properties, which resulted in the present paper.

Let $G = (V, E)$ be a graph with n vertices and m edges and vertex set $V = \{v_1, v_2, \ldots, v_n\}$. We label the vertices of G so that $d_1 \geq d_2 \geq \ldots \geq d_n$, where d_i is the degree of the vertex v_i for $i = 1, 2, \ldots, n$. The average of the degrees of the vertices adjacent to v_i is denoted by μ_i.

In this notation,

$$M_1 = M_1(G) = \sum_{i=1}^{n} (d_i)^2 \quad ; \quad M_2 = M_2(G) = \sum_{v_i v_j \in E} d_i \, d_j \, .$$

The complement of the graph G is denoted by $\bar{G} = (V, \bar{E})$, where $v_i v_j \in \bar{E}$ if and only if $v_i v_j \notin E$. For $i = 1, 2, \ldots, n$, by $\bar{d}_i$ is denoted the degree of the vertex v_i in $\bar{G}$, $\bar{d}_i = n - 1 - d_i$.

The complete graph on n vertices is denoted by K_n. Thus, $\bar{K}_n$ is the n-vertex graph without edges. The graph consisting of disconnected components G_1 and G_2 is denoted by $G_1 \cup G_2$. A tree is a connected graph without cycles. An n-vertex tree possesses $n-1$ edges. The n-vertex tree for which $d_1 = n-1$ is called the star and is denoted by S_n. The n-vertex tree for which $d_1 = 2$ is called the path and is denoted by P_n.

We first state a few immediate results:

$$\begin{aligned}
d_i\,\mu_i &= \text{sum of the degrees of the vertices adjacent to vertex } v_i \\
&= \sum_{v_i v_j \in E} d_j \qquad (1)\\
&\leq 2m - d_i - (n-1-d_i)\,d_n \qquad (2)\\
\sum_{i=1}^{n} d_i\,\mu_i &= \sum_{i=1}^{n} d_i^2 \qquad (3)\\
4\,m^2 &= \left(\sum_{i=1}^{n} d_i\right)^2 = \sum_{i=1}^{n} d_i^2 + 2\sum_{v_i v_j \in E} d_i\,d_j + 2\sum_{v_i v_j \notin E} d_i\,d_j
\end{aligned}$$

i. e.,

$$\sum_{v_i v_j \notin E} d_i\,d_j = 2\,m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i^2 - \sum_{v_i v_j \in E} d_i\,d_j\ . \qquad (4)$$

It is easy to check that $M_2(K_n) = \frac{1}{2}\,n\,(n-1)^3$ and $M_2(\bar{K}_n) = 0$.

By deleting edges from a graph, the second Zagreb index decreases. Thus, the graphs with maximum and minimum M_2 are those with the greatest and smallest number of edges, respectively. This yields:

Theorem 1. *If G is an n-vertex graph, different from K_n and $\bar{K}_n$, then*

$$M_2(\bar{K}_n) < M_2(G) < M_2(K_n)$$

i. e.,

$$0 < M_2(G) < \frac{1}{2}\,n\,(n-1)^3\ .$$

Lemma 2. *The connected n-vertex graph with minimum second Zagreb index is an n-vertex tree.*

Later (in Theorem 11) we demonstrate that the tree with minimum value of M_2 is the path.

Lemma 3. *The following identities are obeyed:*

$$\sum_{v_i v_j \in E} d_i\, d_j = \frac{1}{2} \sum_{i=1}^{n} d_i^2\, \mu_i \tag{5}$$

$$\sum_{v_i v_j \notin E} (d_i + d_j) = 2\,m\,(n-1) - \sum_{i=1}^{n} d_i^2 \tag{6}$$

$$\sum_{v_i v_j \in \bar{E}} \bar{d}_i\, \bar{d}_j = \frac{n(n-1)^3}{2} - 3\,m\,(n-1)^2 + 2\,m^2 + \left(n - \frac{3}{2}\right) \sum_{i=1}^{n} d_i^2 - \sum_{v_i v_j \in E} d_i\, d_j\ . \tag{7}$$

Proof. Bearing in mind Eq. (1), we have

$$\sum_{i=1}^{n} d_i^2\, \mu_i = \sum_{i=1}^{n} d_i \left(\sum_{v_i v_j \in E} d_j \right) = 2 \sum_{v_i v_j \in E} d_i\, d_j$$

which is tantamount to Eq. (5).

In order to deduce Eq. (6) we have

$$2 \sum_{v_i v_j \notin E} (d_i + d_j) = \sum_{i=1}^{n} [(n - 1 - d_i)\, d_i + (2\,m - d_i\, \mu_i - d_i)]$$

i. e.,

$$\sum_{v_i v_j \notin E} (d_i + d_j) = 2\,m\,(n-1) - \sum_{i=1}^{n} d_i^2$$

where Eq. (3) has been employed.

Eq. (7) is obtained as follows:

$$\begin{aligned}
\sum_{v_i v_j \in \bar{E}} \bar{d}_i \bar{d}_j &= \sum_{v_i v_j \notin E} (n - 1 - d_i)(n - 1 - d_j) \\
&= \sum_{v_i v_j \notin E} (n-1)^2 - (n-1) \sum_{v_i v_j \notin E} (d_i + d_j) + \sum_{v_i v_j \notin E} d_i\, d_j \\
&= \frac{n(n-1)^3}{2} - 3\,m\,(n-1)^2 + 2\,m^2 + \left(n - \frac{3}{2}\right) \sum_{i=1}^{n} d_i^2 - \sum_{v_i v_j \in E} d_i\, d_j
\end{aligned}$$

where Eqs. (6) and (4) have been used. □

Note that Eq. (7) can be written also in the form

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

Lemma 4. [9] *Let G be a graph with n vertices and m edges. Then*

$$\sum_{i=1}^{n} d_i^2 \le m \left(\frac{2\,m}{n-1} + n - 2 \right)\ . \tag{8}$$

Lemma 5. [7] *Let G be a graph with n vertices and m edges, $m > 0$. Then the equality*

$$\sum_{i=1}^{n} d_i^2 = m\left(\frac{2m}{n-1} + n - 2\right)$$

holds if and only if G is isomorphic to S_n or K_n or $K_{n-1} \cup K_1$.

Theorem 6. *Let G be a graph with n vertices and m edges. Then the second Zagreb index of G is bounded from above as*

$$M_2(G) \leq 2m^2 - (n-1)\,m\,d_n + \frac{1}{2}(d_n - 1)\,m\left(\frac{2m}{n-1} + n - 2\right) \tag{9}$$

with equality if and only if G is isomorphic to S_n or K_n.

Proof.

$$\begin{aligned}
\sum_{v_i v_j \in E} d_i\, d_j &= \frac{1}{2}\sum_{i=1}^{n} d_i^2\, \mu_i \\
&\leq \frac{1}{2}\sum_{i=1}^{n} d_i\left[2m - d_i - (n-1-d_i)\,d_n\right] && (10)\\
&= 2m^2 - (n-1)\,m\,d_n + \frac{1}{2}(d_n-1)\sum_{i=1}^{n} d_i^2 \\
&\leq 2m^2 - (n-1)\,m\,d_n + \frac{1}{2}(d_n-1)\,m\left(\frac{2m}{n-1} + n - 2\right). && (11)
\end{aligned}$$

Relations (10) and (11) were obtained by taking into account Eqs. (2) and (8), respectively.

Suppose now that equality in (9) holds. Then all inequalities in the above relations become equalities. From (10) we conclude that for every vertex v_i either $d_i = n-1$ or all the vertices v_k not adjacent to v_i are of degree d_n. Then from Eq. (11) and Lemma 5 follows that G is a star or a complete graph.

Conversely, let G be a star or a complete graph. Then it is easily verified that equality holds in (9).

By this the proof of Theorem 6 is completed. □

For the star on n vertices, $d_1 = n-1$, $d_i = 1$, $i = 2,3,\ldots,n$. Therefore $M_2(S_n) = (n-1)^2$.

The inequality (9) holds for all graphs. In the case of trees, $d_n = 1$ and $m = n-1$. Then (9) reduces to $M_2 \leq (n-1)^2$. From these observations we arrive at the following:

Theorem 7. *Let T be a tree with n vertices. If the second Zagreb index of T is maximum, then T is the star.*

An alternative proof of Theorem 7 is in Theorem 8.

Theorem 8. *If T is an n-vertex tree, different from S_n, then $M_2(T) < M_2(S_n)$.*

Proof. Let $\sum\limits_{v_i v_j \in E} d_i d_j$ be maximum. We need to prove that T is the star.

Suppose that v_i is the vertex of the tree T, such that $d_i \mu_i + d_i$ is maximum, where $d_i \mu_i$ is the sum of the degrees of the vertices adjacent to vertex v_i, that is, $d_i \mu_i + d_i \geq d_j \mu_j + d_j$ for all values of j.

We transform T into another tree T^* by choosing one pendant vertex v_k, $k \neq i$, adjacent to v_j, $j \neq i$, deleting the edge $v_k v_j$, and joining the vertices v_i and v_k by an edge. Let the new degree sequence be $d_1^*, d_2^*, \ldots, d_n^*$. Therefore $d_t^* = d_t$ for $t \neq i, j$ whereas $d_i^* = d_i + 1$ and $d_j^* = d_j - 1$.

Two cases are to be distinguished: (i) $v_i v_j \notin E$, and (ii) $v_i v_j \in E$.

Case (i) $v_i v_j \notin E$

$$\begin{aligned}
\sum_{v_i v_j \in E} d_i^* d_i^* - \sum_{v_i v_j \in E} d_i d_j &= [d_i \mu_i + (d_i + 1)] - [d_j \mu_j - 1 + d_j] \\
&= d_i \mu_i + d_i - d_j \mu_j - d_j + 2 > 0 .
\end{aligned}$$

Case (ii) $v_i v_j \in E$:

$$\begin{aligned}
\sum_{v_i v_j \in E} d_i^* d_j^* - \sum_{v_i v_j \in E} d_i d_j &= [d_i \mu_i - d_j + (d_i + 1) + (d_i + 1)(d_j - 1) - d_i d_j] \\
- [d_j \mu_j - 1 - d_i + d_j] &= d_i \mu_i + d_i - d_j \mu_j - d_j + 1 > 0 .
\end{aligned}$$

Thus, in both cases we have

$$\sum_{v_i v_j \in E} d_i^* d_j^* > \sum_{v_i v_j \in E} d_i d_j .$$

i. e., by the above described construction we have increased the value of M_2. If T^* is the star, we are done. If not, then we continue the construction as follows.

It is easy to see that $d_i^* \mu_i^* + d_i^*$ is maximum in T^*, where $d_i^* = d_i + 1$. Next we choose one pendant vertex from T^*, etc. Repeating the procedure sufficient number of times, we arrive at a tree in which the vertex v_i is of degree $n - 1$, i. e., we arrive at S_n. $\square$

Lemma 9. *Let F be a forest with n vertices and m edges. If among forests with n vertices and m edges*

$$\left(n-\frac{3}{2}\right)\sum_{i=1}^{n} d_i^2 - \sum_{v_i v_j \in E} d_i\, d_j$$

is maximum, then F is isomorphic to $S_{m+1} \cup \bar{K}_{n-m-1}$.

Proof. Let v_1 be the highest-degree vertex, of degree d_1. Consider a forest with n vertices and m edges, which is not isomorphic to $S_{m+1} \cup \bar{K}_{n-m-1}$. Then we can take one pendant vertex v_k, $k > 1$, which is adjacent to vertex v_r, $r \neq 1$. We delete the edge $v_k v_r$ and join the vertices v_k and v_1 by an edge. Let the new degree sequence be $d_1^*, d_2^*, \ldots, d_n^*$. Then $d_i^* = d_i$, $i = 2, 3, \ldots, n$, $i \neq r$, $d_1^* = d_1 + 1$, $d_r^* = d_r - 1$.

Two cases arise: (i) $v_1 v_r \notin E$, and (ii) $v_1 v_r \in E$.

Case (i) $v_1 v_r \notin E$:

$$\left[\left(n-\frac{3}{2}\right)\sum_{i=1}^{n}(d_i^*)^2 - \sum_{v_i v_j \in E} d_i^*\, d_j^*\right] - \left[\left(n-\frac{3}{2}\right)\sum_{i=1}^{n} d_i^2 - \sum_{v_i v_j \in E} d_i\, d_j\right]$$

$$\begin{aligned} &\geq (2n-3)(d_1 - d_r) + \sum_{i=1}^{n} d_i - 3 - d_1 m_1 - d_1 + d_r m_r + d_r \\ &= (2n-3)(d_1 - d_r) + \sum_{v_1 v_j \notin E,\, j \neq 1} d_j - 3 + d_r m_r + d_r \,. \end{aligned} \tag{12}$$

Two subcases to be distinguished are (a) $d_r \geq 2$, and (b) $d_r = 1$.

Subcase (a): For $d_r \geq 2$, we can easily see that the expression in (12) is strictly greater than zero.

Subcase (b): For $d_r = 1$,

$$\sum_{v_1 v_j \notin E,\, j \neq 1} d_j \geq 2$$

and $d_r m_r + d_r = 2$. Therefore this expression is strictly greater than zero.

Case (ii) $v_1 v_r \in E$:

$$\left[\left(n-\frac{3}{2}\right)\sum_{i=1}^{n}(d_i^*)^2 - \sum_{v_i v_j \in E} d_i^*\, d_j^*\right] - \left[\left(n-\frac{3}{2}\right)\sum_{i=1}^{n} d_i^2 - \sum_{v_i v_j \in E} d_i\, d_j\right]$$

$$= (2n-3)(d_1 - d_r) + \sum_{v_1 v_j \notin E,\, j \neq 1} d_j - 2 + d_r m_r + d_r \,. \tag{13}$$

In this case, $d_r \geq 2$, and therefore expression (13) is strictly greater than zero.

In both cases we have

$$\left(n-\frac{3}{2}\right)\sum_{i=1}^{n}(d_i^*)^2-\sum_{v_i v_j\in E}d_i^*\,d_j^*>\left(n-\frac{3}{2}\right)\sum_{i=1}^{n}d_i^2-\sum_{v_i v_j\in E}d_i\,d_j\ .$$

Similarly as in Theorem 8, we conclude that F is of the form $S_{m+1}\cup\bar{K}_{n-m-1}$.

Theorem 10. *Let F be a forest with n vertices and m edges. Further, let $M_2(\bar{F})$ be maximum. Then $\bar{F}$ is the complement of $S_{m+1}\cup\bar{K}_{n-m-1}$.*

Proof. Since $\sum_{v_i v_j\in\bar{E}}\bar{d}_i\,\bar{d}_j$ is maximum, from Eq. (7) we conclude that

$$\left(n-\frac{3}{2}\right)\sum_{i=1}^{n}d_i^2-\sum_{v_i v_j\in E}d_i\,d_j$$

is maximum. Theorem 10 follows now from Lemma 9. □

Theorem 11. *If T is an n-vertex tree, different from P_n and S_n, then*

$$M_2(P_n)<M_2(T)<M_2(S_n)\ .$$

Proof. The right–hand side inequality in Theorem 11 has already been verified (in Theorems 7 & 8). In order to prove the left–hand side inequality, we need the following two auxiliary results:

Lemma 12. *Let G be a connected graph, possessing two distinct vertices v_i and v_j, such that a vertex v_x of degree one is attached to v_i and a vertex v_y of degree one is attached to v_j. Let d_i and d_j be the degrees of the vertices v_i and v_j, respectively, in the graph G. Let the graph G^* be obtained from G by deleting the edge $v_x v_i$ and by inserting an edge $v_x v_y$. If $d_i\geq d_j$ then $M_2(G^*)<M_2(G)$. Exceptionally, if $d_i=d_j=2$, and if v_i is adjacent to a vertex of degree 2, then $M_2(G^*)=M_2(G)$.*

Proof. We shall consider the difference $M_2(G)-M_2(G^*)$. For this we need to examine only the contributions coming from edges whose degrees differ in G and G^*. These are the following:

(1) edges adjacent to v_i, different from edge $v_x v_i$

(2) edge $v_y v_j$

(3) edge $v_x v_i$ in G and edge $v_x v_y$ in G^*.

(1): In G the degree of v_i is d_i and the contribution to M_2 of type (1) is $\sum_k d_k\, d_i$. In G^* the degree of v_i is $d_i - 1$ and the contribution to M_2 of type (1) is $\sum_k d_k\,(d_i - 1)$. Recall: $\sum_k$ is summation over vertices adjacent to v_i, different from v_x.

(2): The contribution of edge $v_y\, v_j'$ in G is $1 \times d_j = d_j$. The contribution of edge $v_y\, v_j$ in G^* is $2 \times d_j = 2\, d_j$.

(3): The contribution of edge $v_x\, v_i$ in G is $1 \times d_i = d_i$. The contribution of edge $v_x\, v_y$ in G^* is $1 \times 2 = 2$.

Taking all this into account, we arrive at:

$$\begin{aligned} M_2(G) - M_2(G^*) &= \left[\sum_k d_k\, d_i + d_i + d_j\right] - \left[\sum_k d_k\,(d_i - 1) + 2\,d_j + 2\right] \\ &= \sum_k d_k + d_i - d_j - 2\,. \end{aligned}$$

One vertex attached to v_i must have degree at least two, because the graph G is assumed to be connected. Therefore the term $\sum_k d_k$ is greater than or equal to two. It is equal to two if exactly one vertex (different from v_x) is attached to v_i and if this vertex has degree 2, implying $d_i = 2$. In all other cases this term is greater than 2.

If $d_i \geq d_j$, as assumed, then the term $d_i - d_j - 2$ is greater than or equal to -2. It is equal to -2 if $d_i = d_j$ and is greater than -2 if $d_i > d_j$.

We thus see that the difference $M_2(G) - M_2(G^*)$ is equal to zero if $d_i = d_j = 2$ and if the vertex v_i is adjacent to exactly one vertex of degree 2. In all other cases $M_2(G) - M_2(G^*)$ is greater than zero. □

Lemma 13. *Let G be a connected graph, possessing a vertex v_i to which two vertices, v_x and v_y, of degree one are attached. Let the graph G^* be obtained from G by deleting the edge $v_x\, v_i$ and by inserting an edge $v_x\, v_y$. Then $M_2(G^*) < M_2(G)$. Exceptionally, $M_2(G^*) = M_2(G)$ holds if and only if G does not possess vertices other than v_i, v_x, and v_y.*

Proof is analogous to the proof of Lemma 12, and will not be reproduced here.

Proof of $M_2(P_n) < M_2(T)$. The transformation $G \Rightarrow G^*$, described in Lemmas 12 and 13, either decreases the M_2-value or leaves it unchanged. In the case of trees, both G and G^* possess two vertices of degree one, so one can apply the same transformation to G^*. Repeating the transformation sufficiently many times we ultimately arrive at P_n. □

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