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ON THE UPPER BOUNDS FOR THE FIRST ZAGREB INDEX

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Abstract. The first Zagreb index M_1 is one of the oldest and the most famous topological molecular structure-descriptor, defined as the sum of squares of the degrees of the vertices. In this paper we analyze and compare various upper bounds for the first Zagreb index involving the number of vertices, the number of edges and the maximum and minimum vertex degree. In addition, we propose new upper bound and correct the equality case in [M. Liu, B. Liu, *New sharp upper bounds for the first Zagreb index*, MATCH Commun. Math. Comput. Chem. **62** (2009) 689–698.].

1. Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex v is denoted as $deg(v)$. Specially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called the maximum and minimum degree of G, respectively.

The first Zagreb index is one of the oldest and most used molecular structure-descriptor, defined as the sum of squares of the degrees of the vertices

$$M_1(G) = \sum_{v \in V} deg(v)^2.$$

Zagreb index was first introduced in [7] and the survey of properties of M_1 is given in [17], [19]. Recently, there was a vast research on comparing Zagreb indices [1], [8], [9], [12], establishing various upper and lower bounds [2], [3], [10], [11], [20], [22], and relations involving other graph invariants [5], [13], [21], [23]. For a survey on the first Zagreb index see [6].

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In this paper we classify the upper bounds for the first Zagreb index involving n, m, Δ and δ. We correct the equality case for Theorem 2.3 and Corollary 2.3 from [10] in Section 2, and introduce new sharp upper bound in Section 4. In Section 5 we present the computational results for the four upper bounds, and conclude that the new upper bound

$$M_1(G) \leq 2m(\Delta+\delta) - n\Delta\delta - (n-k)(\Delta-\delta-1),$$

where k is the number of vertices having degree equal to Δ or δ, is the best one.

2. Correction of equality case

We will correct the equality case in Theorem 2.3 from [10], using the Pólya–Szegö inequality [15].

Theorem 2.1. *Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be positive real numbers such that for $1 \leq i \leq n$ holds $a \leq a_i \leq A$ and $b \leq b_i \leq B$, with $a < A$ and $b < B$. Then,*

$$\left(\sum_{i=1}^{n} a_i^2\right) \cdot \left(\sum_{i=1}^{n} b_i^2\right) \leq \frac{1}{4}\left(\sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}}\right)^2 \cdot \left(\sum_{i=1}^{n} a_i b_i\right)^2.$$

The equality holds if and only if the numbers

$$p = \frac{\frac{A}{a}}{\frac{A}{a}+\frac{B}{b}} \cdot n \qquad \text{and} \qquad q = \frac{\frac{B}{b}}{\frac{A}{a}+\frac{B}{b}} \cdot n$$

are integers, $a_1 = a_2 = \ldots = a_p = a$, $a_{p+1} = a_{p+2} = \ldots = a_n = A$, $b_1 = b_2 = \ldots = b_p = B$ and $b_{q+1} = b_{q+2} = \ldots = b_n = b$.

By extending the proof of Theorem 2.1, if we allow $a = A$ or $b = B$, the equality holds also if $AB = ab$, i. e. $a_1 = a_2 = \ldots = a_n = a = A$ and $b_1 = b_2 = \ldots = b_n = b = B$.

Bidegreed graph is a graph whose vertices have exactly two degrees Δ and δ [16].

Theorem 2.2. *Let G be a simple graph with n vertices and m edges. Then*

$$M_1(G) \leq \frac{(\Delta+\delta)^2}{n\Delta\delta} m^2,$$

with equality if and only if G is regular graph, or G is bidegreed graph such that $\Delta+\delta$ divides δn and there are exactly $p = \frac{\delta n}{\Delta+\delta}$ vertices of degree Δ and $q = \frac{\Delta n}{\Delta+\delta}$ vertices of degree δ.

Proof. By setting the values $a_i = 1$ and $b_i = deg(v_i)$ in Theorem 2.2, we have

$$\sum_{i=1}^{n} 1^2 \cdot \sum_{i=1}^{n} deg(v_i)^2 \leq \frac{(AB+ab)^2}{4ABab} \cdot \left(\sum_{i=1}^{n} deg(v_i) \cdot 1\right)^2.$$

Since $A = a = 1$, $B = \Delta$ and $b = \delta$, it follows

$$n \cdot M_1(G) \leq \frac{(\Delta+\delta)^2}{4\Delta\delta} \cdot (2m)^2,$$

which completes the proof. The equality holds if and only if the graph is regular, or bidegreed such that the number

$$p = \frac{n}{1+\frac{\Delta}{\delta}} = \frac{n\delta}{\Delta+\delta}$$

is integer. In the later case, the number of vertices with degree $B = \Delta$ must be exactly p and the number of vertices with degree δ must be exactly $q = \frac{n\Delta}{\Delta+\delta} = n - p$. □

Corollary 2.1. *Let G be a connected (n, m) graph. If $\delta = 1$, then*

$$M_1(G) \leq \frac{nm^2}{n-1},$$

with equality if and only if $G \cong S_n$. If $\delta \geq 2$, then

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

with equality if and only if $G \cong K_3$.

Proof. Obviously the function $f(x) = x + \frac{1}{x}$ is increasing for $x \geq 1$. We will use the upper bound from Theorem 2.2 in the form

$$M_1(G) \leq \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2\right)\frac{m^2}{n}.$$

Case $\delta = 1$**.** Since $1 \leq \frac{\Delta}{\delta} \leq n-1$, we have $M_1(G) \leq (n - 1 + \frac{1}{n-1} + 2)\frac{m^2}{n}$, with equality if and only if G is bidegreed graph with $\Delta = n-1$ and $\delta = 1$, or equivalently $G \cong S_n$.

Case $\delta \geq 2$**.** Since $1 \leq \frac{\Delta}{\delta} \leq \frac{n-1}{2}$, we have $M_1(G) \leq (\frac{n-1}{2} + \frac{2}{n-1} + 2)\frac{m^2}{n}$, with equality if and only if G is regular with $\delta = 2$, or bidegreed graph with $\Delta = n-1$ and $\delta = 2$ and $(n - 1 + 2) \mid 2n$. It follows that equality holds only for K_3, since $n + 1 \mid 2n$ holds only of $n = 1$. □

The authors in [10] claimed that the equality in Theorem 2.2 is achieved if and only if G is regular graph. The obvious counterexample is the star S_n with

$$M_1(S_n) = n(n-1) = \frac{(n-1+1)^2}{n(n-1)\cdot 1}(n-1)^2.$$

Other counterexamples are complete bipartite graphs $K_{p,q}$ with $p+q=n$. Similarly, the authors in [10] claimed that the equality in Corollary 2.1 is achieved if and only if $G \cong K_2$ or $G \cong K_3$, respectively. The obvious counterexample for the first part is the star S_n.

3. New sharp upper bound for $M_1(G)$

We will use the following Diaz-Metcalf inequality [15], in order to present a simple proof for the upper bound established by Das in [2].

Theorem 3.1. *If a_k and b_k, $k = 1, 2, \ldots, n$ are real numbers such that $ma_k \leq b_k \leq Ma_k$ for $k = 1, 2, \ldots, n$, then*

$$\sum_{k=1}^{n} b_k^2 + mM \sum_{k=1}^{n} a_k^2 \leq (M+m) \sum_{k=1}^{n} a_k b_k.$$

The equality holds if and only if either $b_k = ma_k$ or $b_k = Ma_k$ for every $k = 1, 2, \ldots, n$.

Theorem 3.2. *Let G be a simple graph with n vertices and m edges. Then*

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta, \tag{3.1}$$

with equality if and only if G is regular or bidegreed graph.

Proof. By setting $b_i = deg(v_i)$ and $a_i = 1$ in Theorem 3.1, the inequality follows since $\delta \cdot 1 \leq b_i \leq \Delta \cdot 1$. □

Remark 3.1. The bound from Theorem 3.2 is always better than the bound from Theorem 2.2,

$$\frac{(\Delta+\delta)^2}{n\Delta\delta} m^2 \geq 2m(\Delta+\delta) - n\Delta\delta.$$

Using the arithmetic-geometric inequality we get

$$\frac{(\Delta+\delta)^2}{n\Delta\delta} m^2 + n\Delta\delta \geq 2\sqrt{\frac{(\Delta+\delta)^2}{n\Delta\delta} m^2 \cdot n\Delta\delta} = 2m(\Delta+\delta),$$

with equality if and only if $(\Delta+\delta)m = n\Delta\delta$.

For $\delta = 1$, it follows

$$M_1(G) \leq \Delta(2m - n) + 2m.$$

Similarly as in Section 6 of [10], one can determine the first four largest $M_1(G)$ in the class of trees on n vertices. For $\Delta \leq n-5$, it follows $M_1(G) \leq n^2-5n+8 < n^2-5n+14$.

Using the same technique, we can derive the following stronger inequality

Theorem 3.3. *Let G be a simple non-regular graph with n vertices and m edges, with a vertices of degree maximal Δ and b vertices of degree δ. Then*

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta - (n - a - b)(\Delta - \delta - 1), \tag{3.2}$$

with equality if and only if the vertex degrees are equal to δ, $\delta + 1$, $\Delta - 1$ or Δ.

Proof. For the vertices v_i, such that $\delta < deg(v_i) < \Delta$ it holds

$$\Delta - \delta - 1 \leq (\Delta - deg(v_i))(deg(v_i) - \delta) = -deg(v_i)^2 - \Delta\delta + deg(v_i)(\Delta + \delta),$$

with equality if and only if $deg(v_i) = \delta + 1$ or $deg(v_i) = \Delta - 1$. After adding these inequalities, we get

$$(n-a-b)(\Delta-\delta-1) \leq -\sum_{\delta<deg(v_i)<\Delta} deg(v_i)^2 - (n-a-b)\Delta\delta + (2m-a\Delta-b\delta)(\Delta+\delta),$$

and finally

$$M_1(G) \leq a\Delta^2+b\delta^2+(n-a-b)(\Delta-\delta-1)-n\Delta\delta+(a+b)\Delta\delta+2m(\Delta+\delta)-(a\Delta+b\delta)(\Delta+\delta)$$

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta - (n - a - b)(\Delta - \delta - 1)$$

The equality holds if and only if $deg(v_i) \in \{\delta, \delta + 1, \Delta - 1, \Delta\}$. This completes the proof. $\square$

In particular, the equality holds for all chemical graphs (with maximum degree $\Delta \leq 4$).

Let $\overline{G}$ denote the complement of a graph G. Next we will establish the Nordhaus–Gaddum type inequalities [18] for $M_1(G)$.

Theorem 3.4. *Let G be a simple graph with n vertices and m edges, with a vertices of degree maximal Δ and b vertices of degree δ. Then*

$$M_1(G)+M_1(\overline{G}) \leq n(n-1)^2-2n\delta\Delta+4m(1+\delta+\Delta-n)-2(\Delta-\delta-1)(n-a-b), \tag{3.3}$$

with equality if and only if the vertex degrees of G are equal to δ, $\delta + 1$, $\Delta - 1$ or Δ.

Proof. The complement graph $\overline{G}$ has $\frac{n(n-1)}{2} - m$ edges, maximal degree $n-1-\delta$ and minimal degree $n-1-\Delta$. Therefore,

$$M_1(\overline{G}) \leq 2\left(\frac{n(n-1)}{2} - m\right)(2n-2-\delta-\Delta) - n(n-1-\delta)(n-1-\Delta) - (n-a-b)(\Delta-\delta-1).$$

By adding this inequality with the relation (3.2), we complete the proof.
The equality holds if and only if $deg(v_i) \in \{\delta, \delta+1, \Delta-1, \Delta\}$ as in the proof of Theorem 3.3. $\square$

The second Zagreb index (see [4] and [9]) is defined as the sum of product of the degrees of adjacent vertices

$$M_2(G) = \sum_{uv \in E} deg(v) \cdot deg(u).$$

We will use the following estimation from [3]

$$M_2(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)M_1(G),$$

with equality if and only if G is a regular graph or G is bidegreed graph in which each vertex is of degree either δ or $\Delta = n-1$.

Theorem 3.5. *Let G be a simple graph with n vertices and m edges, with a vertices of degree maximal Δ and b vertices of degree δ. Then*

$$M_2(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)\left(2m(\Delta+\delta) - n\Delta\delta - (n-a-b)(\Delta-\delta-1)\right),$$

with equality if and only if G is a regular graph or G is bidegreed graph in which each vertex is of degree either δ or $n-1$.

4. Computational results

In this section, we compare four upper bounds for the first Zagreb index.

Theorem 4.1. [2] *Let G be a connected graph with n vertices, m edges, maximum degree Δ, and minimum degree δ. Then*

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

with equality if and only if G is a star or a regular graph.

Theorem 4.2. [10] *Let G be a connected graph with n vertices, m edges, maximum degree Δ, and minimum degree δ. Then*

$$M_1(G) \leq \max\left\{ m\left(\Delta + \delta - 1 + \frac{2m - \delta(n-1)}{\Delta}\right), m\left(\delta + 1 + \frac{2m - \delta(n-1)}{2}\right) \right\}.$$

Equality can be obtained, for example, by a star or a regular graph of order $n \geq 3$.

Theorem 4.3. [3] *Let G be a graph with $n > 1$ vertices, m edges, maximum degree Δ, second maximum degree Δ' and minimum degree δ. Then*

$$M_1(G) \leq \Delta^2 + (\Delta' + \delta)(2m - \Delta) - (n-1)\Delta'\delta.$$

Equality holds if and only if G is isomorphic to a graph H, such that for the vertex degrees of H holds $deg(v_1) = \Delta$, $deg(v_2) = deg(v_3) = \ldots = deg(v_p) = \Delta'$ and $deg(v_{p+1}) = deg(v_{p+2}) = \ldots = deg(v_n) = \delta$, for some $2 \leq p \leq n$.

In Table 1 and Table 2 we present the computational results for connected graphs on $n = 3$ to $n = 10$ vertices and trees on $n = 10$ to $n = 20$ vertices. The first three columns contain n, the number of connected graphs (trees) on n vertices and the average value of the first Zagreb index $M_1(G)$. The next four groups of three columns represent the average value of the upper bound, the standard deviation ($\sqrt{\frac{\sum_G (X(G) - M_1(G))^2}{count}}$) and the number of graphs for which the equality holds.

By comparing these values, it is clear that the upper bound (3.2) has the smallest deviation from the first Zagreb index. For the standard benchmark data sets of chemical compounds proposed by the International Academy of Mathematical Chemistry [14], it can be easily observed that the proposed upper bound from Theorem 3.3 is superior in comparison with the other upper bounds. In particular, for all octanes (see Figure 1) we have the equality in Theorem 3.3.

Parameters			Theorem 3.3			Theorem 4.1			Theorem 4.2			Theorem 4.3		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	9.000	9.000	0.000	2	9.000	0.000	2	9.000	0.000	2	9.000	0.000	2
4	6	19.667	19.667	0.000	6	19.833	0.408	5	19.667	0.000	6	19.667	0.000	6
5	21	35.429	35.429	0.000	21	37.524	2.600	3	37.476	2.535	3	35.714	0.690	17
6	112	55.661	55.786	0.582	106	60.938	6.007	6	62.393	8.255	6	56.893	2.146	62
7	853	82.626	83.198	1.587	683	93.980	11.998	5	100.733	21.114	5	85.931	4.762	230
8	11117	118.451	120.045	3.345	6658	138.211	20.598	18	156.795	43.717	18	124.923	8.499	1240
9	261080	166.106	169.483	5.997	105659	197.810	32.525	23	237.814	79.747	23	176.949	13.485	10231
10	11716571	227.502	233.545	9.682	3012950	274.469	48.007	168	349.074	133.191	168	243.883	19.720	147451

TABLE 1. Comparing the upper bounds for first Zagreb index for small graphs.

Parameters			Theorem 3.3			Theorem 4.1			Theorem 4.2			Theorem 4.3		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	44.585	44.802	0.622	91	64.764	20.786	1	60.113	16.538	1	46.434	2.395	33
11	235	50.026	50.379	0.892	189	75.519	26.225	1	71.485	22.168	1	52.668	3.190	47
12	551	55.401	55.922	1.194	413	86.192	31.719	1	83.348	29.048	1	58.927	4.082	65
13	1301	60.764	61.477	1.530	913	97.267	37.644	1	96.874	36.824	1	65.203	5.029	91
14	3159	66.129	67.056	1.890	2075	108.412	43.679	1	110.742	45.765	1	71.569	6.096	123
15	7741	71.495	72.658	2.278	4774	119.733	49.997	1	126.456	55.660	1	77.990	7.238	170
16	19320	76.860	78.278	2.686	11214	131.351	56.418	1	142.377	66.657	1	84.498	8.483	219
17	48629	82.230	83.924	3.118	26619	143.068	63.039	1	160.224	78.637	1	91.081	9.805	303
18	123867	87.603	89.589	3.567	64057	154.885	69.768	1	178.177	91.672	1	97.750	11.209	391
19	317955	92.979	95.277	4.036	155575	166.852	76.646	1	198.105	105.704	1	104.492	12.678	536
20	823065	98.358	100.984	4.522	381521	178.522	83.629	1	218.081	120.762	1	111.307	14.211	669

TABLE 2. Comparing the upper bounds for first Zagreb index for small trees.

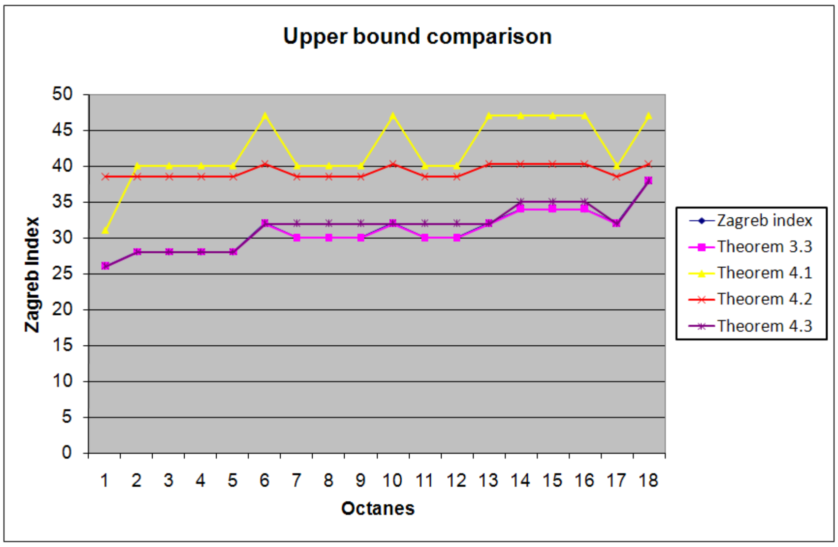

FIGURE 1. The comparison of upper bounds for the first Zagreb index on the set of 18 octanes.

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