SCIENTIFIC PUBLICATIONS OF THE STATE UNIVERSITY OF NOVI PAZAR
SER. A: APPL. MATH. INFORM. AND MECH. vol. 8, 1 (2016), 11-19.

New Sharp Lower Bounds for the First Zagreb Index

T. Mansour, M. A. Rostami, E. Suresh, G. B. A. Xavier

Abstract: The first Zagreb index $M_1(G)$ is defined as the sum of squares of the degrees of the vertices. In this paper we compare and analyze numerous lower 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 lower bound and correct the equality case in [E.I. Milovanović and I.Ž. Milovanović, Sharp Bounds for the first Zagreb index and first Zagreb coindex, Miskolc Mathematical notes, 16 (2015) 1017-1024].

Keywords: First Zagreb index, second Zagreb index, inverse degree.

1 Introduction

All graphs under discussion are finite, undirected and simple. Let $G = (V,E)$ be a simple graph with n vertices and m edges. The degree of the vertex v_i $(1 \leq i \leq n)$ is denoted by $d(v_i)$ such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. As usual, δ and Δ denote the minimum and the maximum vertex degree of G. The second maximum vertex degree is denoted by Δ_2.

In 1987, the inverse degree was first appeared through conjectures of the computer program Graffiti [7]. The inverse degree of a graph G with no isolated vertices are defined as $ID(G) = \sum_{v\in V(G)} \frac{1}{d(v)}$. For the recent results of the inverse degree, refer [2, 11]. In 1972, Gutman and Trinajstić [8] explored the study of total π-electron energy on the molecular structure and introduced two vertex degree-based graph invariants. These invariants are defined as $M_1(G) = \sum_{v\in V(G)} d(v)^2$ and $M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$. One of the most important and common mathematical property of these invariants are studying the bounds for the graphs. For the recent improvements of these bounds see [4, 10] and the references are cited therein. These bounds as usual depends on their structural variables (n, m, Δ, δ and similar).

Manuscript received December 21, 2015; accepted March 1, 2016.

T. Mansour is with the University of Haifa, 3498838 Haifa, Israel; M. A. Rostami is with the Institute for Computer Science, Friedrich Schiller University Jena, Germany; E. Suresh is with the Velammal Engineering College, Surapet, Chennai-66, Tamil Nadu, India; G. B. A. Xavier is with the Sacred Heart College, Tirupattur-635601, Tamil Nadu, India.

In chemical and mathematical literature numerous upper bounds are obtained for the Zagreb indices, however only very few lower bounds are discovered. This motivates the authors to propose some new lower bounds for the first Zagreb index involving the new parameter inverse degree $ID(G)$ with n, m, Δ, Δ_2 and δ. In addition, we compare and analyze our results with the existing lower bounds in the literature so far. Finally, we conclude that our results are stronger and are the improvement of the existing results.

2 Preliminaries

A bidegreed graph is a graph whose vertices have exactly two degrees Δ and δ. Let Γ be the class of graphs such that $d(v_i) = \delta$, $i = 2, 3, \ldots, n$. Γ is the special case of the Bidegreed graphs. Let Γ_2 and Γ_3 be the class of graphs, such that $d(v_2) = \cdots = d(v_{n-1}) = \Delta_2$, $d(v_n) = \delta$ with $d(v_1) > d(v_i), i = 2, 3, \ldots, n$ and $d(v_i) = \delta$ with $d(v_1) \geq d(v_2) > d(v_i), i = 3, 4, \ldots, n$ respectively.

Next we recall the lower bounds for the first Zagreb index available in the literature (see [5, 9, 12, 6]).

Lemma 1. *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \geq \frac{4m^2}{n} \tag{1}$$

equality is attained if and only if G is regular.

In 2003, Das [3] obtained the following lower bound which is better than Lemma 1.

Lemma 2. *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \geq \Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n-2} \tag{2}$$

with equality if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_2$.

In 2015, Das, Xu and Nam [4] also proposed a new improvement for Lemma 1.

Lemma 3. *Let G be a graph of order $n(\geq 3)$, m edges with maximum degree Δ, second maximum degree Δ_2 and minimum degree δ. Then*

$$M_1(G) \geq \Delta^2 + \frac{(2m - \Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\Delta_2 - \delta)^2 \tag{3}$$

with equality if and only if G is regular or $G \in \Gamma$.

3 Correction of equality case

Very recently, E.I. Milovanović and Ž. Milovanović [10] have proposed a new lower bound for the first Zagreb index. In addition, it was proved that Lemma 4 is better than Lemma 1.

Lemma 4. *Let G be a graph of order $n(\geq 2)$ and m edges. Then*

$$M_1(G) \geq \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2 \tag{4}$$

with equality if and only if G is isomorphic with k-regular graph, $1 \leq k \leq n-1$.

Remark: At first, the conclusion which relates to the equality case of (4) is wrong, which we intent to complete the equality case in Lemma 4. The equality of (4) holds for the graphs other than $k-$ regular graphs (See Graphs G_1 and G_2 of Fig. 1).

Let G be a graph with vertex degrees $d(v_1) = \delta + 2$, $d(v_2) = \cdots = d(v_{n-1}) = \delta + 1$ and $d(v_n) = \delta$. Then

$$2m = \sum_{i=1}^{n} d(v_i) = n(\delta + 1)$$

$$M_1(G) = \sum_{i=1}^{n} d(v_i)^2 = (\delta + 2)^2 + (n-2)(\delta + 1)^2 + \delta^2 = n(\delta + 1)^2 + 2$$

from the inequality (4), we have

$$\frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2 = \frac{1}{n} n(\delta + 1) n(\delta + 1) + \frac{1}{2}(\delta + 2 - \delta)^2 = n(\delta + 1)^2 + 2$$

this completes that the equality of (4) holds for the above case. Conversely, it is easy to see that, if the equality holds in (4), then G has the vertex degrees $d(v_1) = \delta + 2$, $d(v_2) = \cdots = d(v_{n-1}) = \delta + 1$ and $d(v_n) = \delta$.

Similarly, the equality of (4) holds for the graphs with even order, whose vertex degrees are $d(v_1) = 2k+3$, $d(v_2) = \cdots = d(v_{n-1}) = 2k+1$ and $d(v_n) = 2k-1$ with $k \geq 1$. In addition, equality holds for $d(v_1) = 2k+4$, $d(v_2) = \cdots = d(v_{n-1}) = 2k+2$ and $d(v_n) = 2k$. In the same intuition one can conjecture that the equality of (4) holds for all graphs with vertex degrees $d(v_2) = \cdots = d(v_{n-1})$, it is not true in general (Refer Graph G_3 of Fig. 1).

Finally we conclude, the equality of (4) also holds if and only if $d(v_1) = \Delta$, $d(v_2) = \cdots = d(v_{n-1}) = \Delta - k$ and $d(v_n) = \delta$ for some $0 < k < \Delta - \delta$. Thus, it is easy to see that the bound in (2) is always better than (4) and so we left the proof to the interested reader.

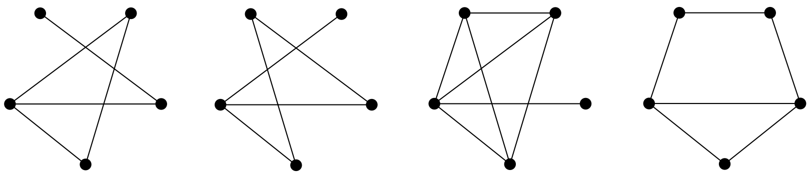

Fig. 1. Graphs on 5 vertices.

4 Lower Bounds on First Zagreb index

Now, our aim is to improve the existing bounds and as well as to give some new lower bounds for the first Zagreb index in terms of n, m, Δ, Δ_2 and δ. At first we improve the classical lower bound proposed in Lemma 1.

Theorem 1. *Let G be a simple graph of order $n (\geq 3)$. Then*

$$M_1(G) \geq \Delta^2 + \Delta_2^2 + \frac{(2m - \Delta - \Delta_2)^2}{(n-2)} \tag{5}$$

equality holds if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_3$.

Proof. Let $a_1, a_2, \ldots, a_r$ and $b_1, b_2, \ldots, b_r$ be any two sequences of real numbers, then by Cauchy-Schwartz inequality, we get

$$\sum_{i=1}^{r} a_i^2 \sum_{i=1}^{r} b_i^2 \geq \left(\sum_{i=1}^{r} a_i b_i \right)^2 . \tag{6}$$

If we set $r = n-2, a_i = d(v_{i+2})$ and $b_i = 1$, for all $i = 1, 2, \cdots, r$, in the above, and using

$$\sum_{i=3}^{n} d(v_i) = 2m - \Delta - \Delta_2 \quad \text{and} \quad \sum_{i=3}^{n} d(v_i)^2 = M_1^2(G) - \Delta^2 - \Delta_2^2, \tag{7}$$

we get the required inequality. Suppose $G \in \Gamma_3$, then $d(v_i) = \delta$, for $i = 3, 4, \ldots, n$. So $(n-2)\delta = 2m - \Delta - \Delta_2$ and $M_1^2(G) = \Delta^2 + \Delta_2^2 + (n-2)\delta^2$. Next, if $G \in \Gamma$, then $d(v_2) = \Delta_2 = \delta$. So it is easy to see that if $G \in \Gamma$ or G is regular, then equality holds.

Conversely, if the equality of (5) holds, then $\sum_{i=3}^{n} d(v_i)^2 = \frac{(2m-\Delta-\Delta_2)^2}{(n-2)}$. Using the equality condition of (1), we conclude that $d(v_i) = \delta$, for $i = 3, 4, \cdots, n$ and $d(v_1) \geq d(v_2) > \delta$, that is, $G \in \Gamma$ or $G \in \Gamma_3$. □

Corollary 1. *With the assumptions in Theorem 1, one has the inequality*

$$M_1(G) \geq \Delta^2 + \frac{(2m - \Delta)^2}{(n-1)} \tag{8}$$

equality holds if and only if G is regular or $G \in \Gamma$.

Remark 1. *For any graph G, the lower bound* (5) *to be better than* (1)*. In order to prove this, first we have to show that* (8) *is better than* (1)*. Suppose, we assume that*

$$\Delta^2 + \frac{(2m-\Delta)^2}{n-1} \leq \frac{4m^2}{n},$$

that is

$$n(n-1)\Delta^2 + (2m-\Delta)^2 \geq 4m^2(n-1) \Rightarrow (2m-n\Delta)^2 \leq 0,$$

which leads to the contradiction and which fulfill our claim. Next, by Root Mean Square - Geometric Mean inequality, the following inequality is always true,

$$(n-1)^2\Delta_2^2 + (2m-\Delta)^2 \geq 2(n-2)\,(2m-\Delta)\,\Delta_2,$$

that is

$$(n-1)(n-2)\Delta_2^2 + (n-1)(2m-\Delta-\delta)^2 \geq (n-2)(2m-\Delta)^2.$$

Thus

$$\Delta^2 + \Delta_2^2 + \frac{(2m-\Delta-\Delta_2)^2}{(n-2)} \geq \Delta^2 + \frac{(2m-\Delta)^2}{(n-1)},$$

which completes our claim.

The lower bounds in (2) and (5) are incomparable. Namely, there exist molecular graph $1,1$-diethylcyclobutane for which (2) is better than (5), and for $1,2$-diethylcyclobutane (5) is better than (2). It is interesting to see that for $1,1$-dimethylcyclopropane, the lower bounds in (2) and (5) coincides together, other than equality case.

Theorem 2. *Let G be a simple graph of order* $n(\geq 3)$ *with no isolated vertices. Then*

$$M_1^2(G) \geq \Delta^2 + \Delta_2^2 + \frac{(2m-\Delta-\Delta_2)^2}{n-2} + \frac{(2m-\Delta-\Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right)}{n-2} - (n-2), \qquad (9)$$

and equality holds if and only if G is regular or $G \in \Gamma$ *or* $G \in \Gamma_3$.

Proof. Consider $w_1, w_2, \ldots, w_r$ be the non-negative weights, then we have the weighted version of the Cauchy-Schwartz inequality

$$\sum_{i=1}^{r} w_i a_i^2 \sum_{i=1}^{r} w_i b_i^2 \geq \left(\sum_{i=1}^{r} w_i a_i b_i\right)^2. \qquad (10)$$

Since w_i is non-negative, we assume that $w_i = x_i - y_i$ with $x_i \geq y_i \geq 0$. So, we get

$$\sum_{i=1}^{r} x_i a_i^2 \sum_{i=1}^{n} x_i b_i^2 - \left(\sum_{i=1}^{r} x_i a_i b_i\right)^2 \geq \sum_{i=1}^{r} y_i a_i^2 \sum_{i=1}^{r} y_i b_i^2 - \left(\sum_{i=1}^{r} y_i a_i b_i\right)^2 \geq 0.$$

If we set $r = n-2$, $a_i = d(v_{i+2})$ and $b_i = 1$, $i = 1,2,\ldots,r$, and since G has no isolated vertices, then we have $\frac{1}{d(v_i)} \leq 1, \forall v_i \in V(G)$. so fix $x_i = 1, y_i = \frac{1}{d(v_i)}$ in the above, we get

$$(n-2)\sum_{i=3}^{n} d(v_i)^2 - \left(\sum_{i=3}^{n} d(v_i)\right)^2 \geq \sum_{i=3}^{n} d(v_i) \sum_{i=3}^{n} \frac{1}{d(v_i)} - (n-2)^2 \geq 0 \qquad (11)$$

$$\left(M_1^2(G) - \Delta^2 - \Delta_2^2\right)(n-2) \geq (2m - \Delta - \Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right) + (2m - \Delta - \Delta_2)^2 - (n-2)^2.$$

The equality case follows the similar argument of Theorem 1, which completes our claim. □

Corollary 2. *With the assumptions in Theorem 2, one has the inequality*

$$M_1^2(G) \geq \Delta^2 + \delta^2 + \frac{(2m-\Delta-\delta)^2}{n-2} + \frac{(2m-\Delta-\delta)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)}{n-2} - (n-2), \qquad (12)$$

and equality holds if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_2$.

Remark 2. *Utilizing the inequality* (11), *we get*

$$(2m - \Delta - \Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right) \geq (n-2)^2,$$

this concludes that for any graph G with $n(\geq 3)$, our lower bound (9) *is always better than the lower bound* (5)*. In analogy, also we conclude that the lower bound in* (12) *is stronger than* (2)*.*

It is interesting to see that, the lower bounds in (3) and (9) are incomparable. For the graph G_1, the lower bound in (9) is better than (3) and for G_4, the lower bound in (3) is better than (9), depicted in Fig. 1.

Theorem 3. *Let G be a simple graph of order $n(\geq 3)$ with no isolated vertices. Then*

$$M_1^2(G) \geq \Delta^2 + \Delta_2^2 + \Psi_1^* \qquad (13)$$

equality holds if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_3$,

$$\text{where } \Psi_1^* = \frac{\left((2(m+1) - n - \Delta - \Delta_2) + \sqrt{(2m-\Delta-\Delta_2)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\Delta_2}\right)}\right)^2}{n-2}.$$

Proof. Using (10), one can get

$$\left(\sum_{i=1}^{n} x_i a_i^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^{n} x_i b_i^2\right)^{\frac{1}{2}} - \sum_{i=1}^{n} x_i a_i b_i \geq \left(\sum_{i=1}^{n} y_i a_i^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^{n} y_i b_i^2\right)^{\frac{1}{2}} - \sum_{i=1}^{n} y_i a_i b_i \geq 0,$$

the rest of the proof follows from the same terminology of the Theorem 2. □

Corollary 3. *With the assumptions in Theorem 2, one has the inequality*

$$M_1^2(G) \geq \Delta^2 + \delta^2 + \Psi_2^*, \tag{14}$$

and equality holds if and only if G is regular or $G \in \Gamma$ or $G \in \Gamma_2$,

$$\text{where } \Psi_2^* = \frac{\left((2(m+1) - n - \Delta - \delta) + \sqrt{(2m - \Delta - \delta)\left(ID(G) - \frac{1}{\Delta} - \frac{1}{\delta}\right)}\right)^2}{n-2}$$

Remark 3. *Our bound given by* (13) *is always better than* (3)*. In order to prove this, we have to show that*

$$\Delta^2 + \Delta_2^2 + \Psi_1^* \geq \Delta^2 + \frac{(2m-\Delta)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}\left(\Delta_2^2 + \delta^2 - 2\Delta_2\delta\right).$$

By direct observation we have, $2\Delta_2\delta > \delta^2$,

$$\Delta^2 + \frac{(2m-\Delta)^2}{n-2} > \Delta^2 + \frac{(2m-\Delta)^2}{n-1} \text{ and } \frac{(n-1)}{(n-2)}\Delta_2^2 > \frac{2(n-2)}{(n-1)^2}\Delta_2^2.$$

using the above results, we complete our claim.

5 Computational Results

In this section, we compare five lower bounds for the first Zagreb index. For computational purpose, we used GraphTea[1], a software tool focusing on extracting information and visualization on graphical problems. It offers powerful ways to query or directly interact with properties of a particular instance of a graphical problem. It is specially designed for analyze properties of topological indices.

In Table 1, we present the computational results for connected graphs on $n = 3$ to $n = 9$ 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 lower bound, the standard deviation $\sqrt{\frac{\sum_G (M_1(G) - X(G))^2}{vertex\ count}}$ and the number of graphs for which the equality holds.

On comparing these values along with the Remark 3, we conclude that our bounds (13) and (14) has the smallest deviation from the first Zagreb index and are stronger than the existing results so far in the literature.

Parameters			Theorem 3			Corollary 3			Lemma 3			Lemma 4		
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	8.917	0.118	1
4	6	19.667	19.645	0.053	5	19.596	0.131	4	19.556	0.157	3	19.333	0.500	3
5	21	35.429	35.237	0.293	9	35.149	0.488	9	34.893	0.708	5	34.543	1.189	4
6	112	55.661	55.064	0.832	22	54.896	1.101	19	54.186	1.818	7	53.908	2.214	13
7	853	82.626	81.314	1.668	47	81.114	1.953	52	79.745	3.419	17	79.682	3.552	14
8	11117	118.451	116.078	2.852	176	115.837	3.155	181	113.677	5.501	36	113.991	5.221	111
9	261080	166.106	162.259	4.437	657	162.043	4.711	890	159.008	8.004	136	159.804	7.203	301
10	106	44.585	43.757	1.063	5	42.723	2.406	1	40.770	4.232	1	37.999	7.665	0
11	235	50.026	48.919	1.374	5	47.747	2.836	1	45.312	5.150	1	42.400	8.749	0
12	551	55.401	53.973	1.715	6	52.615	3.420	1	49.654	6.235	1	46.667	9.908	0
13	1301	60.764	58.992	2.077	6	57.504	3.920	1	54.008	7.270	1	50.951	11.006	0
14	3159	66.129	63.993	2.458	7	62.349	4.495	1	58.300	8.385	1	55.188	12.164	0
15	7741	71.495	68.982	2.850	7	67.203	5.034	1	62.598	9.481	1	59.429	13.303	0
16	19320	76.860	73.956	3.260	8	72.032	5.611	1	66.861	10.620	1	63.642	14.478	0
17	48629	82.230	78.924	3.683	8	76.866	6.178	1	71.124	11.757	1	67.853	15.653	0
18	123867	87.603	83.882	4.120	9	81.687	6.763	1	75.370	12.917	1	72.050	16.849	0
19	317955	92.979	88.833	4.569	9	86.506	7.347	1	79.611	14.083	1	76.241	18.051	0
20	823065	98.358	93.776	5.029	10	91.319	7.941	1	83.842	15.261	1	80.422	19.266	0

Table 1. Comparing the lower bounds for graphs up to 9 vertices and trees from 10 to 20 vertices on the first Zagreb index.

References

[1] M. ALI ROSTAMI, H. MARTIN BÜCKER, A. AZADI, *Illustrating a Graph Coloring Algorithm Based on the Principle of Inclusion and Exclusion Using GraphTea*, LNCS, Springer **8719** (2014) 514–517.

[2] M. BIANCHI, A. CORNARO, J.L. PALACIOS, A. TORRIERO, *New bounds of degree-based topological indices for some classes of c-cyclic graphs,* Discrete App. Math. **184** (2015) 62-75.

[3] K. C. DAS, *Sharp bounds for the sum of the squares of the degrees of a graph*, Kragujevac J Math. **25** (2003) 31–49.

[4] K. C. DAS, K. XU, J. NAM, *Zagreb indices of graphs*, Front. Math. China **10** (2015) 567–582.

[5] D. DE CAEN, *An upper bound on the sum of squares of degrees in a graph*, Discrete Math. **185** (1998) 245–248.

[6] C.S. EDWARDS,*The largest vertex degree sum for a triangle in a graph*, Bul. London Math. Soc., **9** (1977) 203–208.

[7] S. FAJTLOWICZ,*On conjectures of graffiti II*, Congr. Numer. **60** (1987) 189–197.

[8] I. GUTMAN, N. TRINAJSTIĆ, *Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972) 535–538.

[9] A. ILIĆ, D. STEVANOVIĆ, *On comparing Zagreb indices*, MATCH Commun. Math. Comput. Chem. **62** (2009) 681–687.

[10] E.I. MILOVANOVIĆ, I.Ž. MILOVANOVIĆ, *Sharp Bounds for the first Zagreb index and first Zagreb coindex*, Miskolc Mathematical notes **16** (2015) 1017–1024.

[11] K. XU, K.C. DAS, *Some extremal graphs with respect to inverse degree*, Discrete App. Math. (2015) http://dx.doi.org/10.1016/j.dam.2015.09.004

[12] B. ZHOU, N. TRINAJSTIĆ, *On general sum-connectivity index*, J. Math. Chem. **47** (2010) 210–218.