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On the Bounds of the First Reformulated Zagreb Index

T. Mansour[1], M. A. Rostami[2], E. Suresh[3,*], G. B. A. Xavier[4]

[1]Department of Mathematics, University of Haifa, 3498838 Haifa, Israel
[2]Institute for Computer Science, Friedrich Schiller University Jena, Germany
[3]Department of Mathematics, Velammal Engineering College, Surapet, Chennai-66, Tamil Nadu, India
[4]Department of Mathematics, Sacred Heart College, Tirupattur-635601, Tamil Nadu, India
*Corresponding author: sureshkako@gmail.com

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Abstract The edge version of traditional first Zagreb index is known as first reformulated Zagreb index. In this paper, we analyze and compare various lower and upper bounds for the first reformulated Zagreb index and we propose new lower and upper bounds which are stronger than the existing and recent results [*Appl. Math. Comp.* **273** (2016) 16-20]. In addition, we prove that our bounds are superior in comparison with the other existing bounds.

Keywords: *Zagreb indices, first reformulated Zagreb index, forgotten topological index*

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1. Introduction

Throughout this paper, we consider finite connected undirected simple graphs. Let G be such a graph with n vertices and m edges. The degree of a vertex u is denoted by $d(u)$. Especially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$ are called as maximum and minimum degree of G, espectively. The degree of an edge is denoted by $d(e)$ in G, which is defined by $d(e) = d(u)+d(v)-2$ for $e = uv \in E(G)$. Let $\overline{G}$ denotes the complement of G, with the same vertex set such that two vertices u and v are adjacent in $\overline{G}$ if and only if they are not adjacent in G.

The first and second Zagreb indices are defined as (for instance, see [9] and references cited therein)

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

$$\text{and } M_2^1(G) = \sum_{uv\in E(G)} d(u)d(v).$$

Numerous papers were recorded in the literature regarding the mathematical and chemical properties on Zagreb indices and the surveys on Zagreb indices. For the recent outcomes on Zagreb indices, see [5] and references cited therein. In 2005, Li and Zheng [13] introduced the the generalized version of the first Zagreb index. For $\alpha \in \mathbb{R}$ and G be any graph, it satisfies

$$M_1^{\alpha+1}(G) = \sum_{v\in V(G)} d(v)^{\alpha+1} = \sum_{uv\in E(G)} \left[d(u)^{\alpha} + d(v)^{\alpha}\right]. \quad (1.1)$$

In 2015, Fortula and Gutman [8] re-introduced the forgotten topological index:

$$F(G) = M_1^3(G) = \sum_{v\in V(G)} d(v)^3.$$

Mathematical properties of the forgotten topological index is seen in [4,8,11,19]. Miličević, Nikolić and Trinajstić [15] reformulated the first Zagreb index in terms of edge-degree instead of vertex-degree:

$$EM_1^2(G) = \sum_{e\in E(G)} d(e)^2.$$

The first reformulated Zagreb index is simply the Zagreb index of its line graph $L(G)$. The use of these descriptors in QSPR study was also discussed in their report [15]. In [6,11,12,17,20], various properties, relations and bounds are also explored.

The inverse degree was first appeared through conjectures of the computer program Graffiti [7] denote by $ID(G)$; with no isolated vertices defined by

$$ID(G) = \sum_{v\in V(G)} \frac{1}{d(v)}.$$

The inverse degree is a special case formula at $\alpha = -1$ in (1.1). For the recent results of the inverse degree, see [3,18]. In analogy, the inverse edge degree of a graph G with no isolated edges is defined by

$$IED(G) = \sum_{e\in E(G)} \frac{1}{d(e)}.$$

This paper is organized as follows. In Section 2, we give some preliminaries and basic definitions that will be used throughout the paper. In Sections 3 and 4, we present lower and upper bounds on the first reformulated Zagreb index $EM_1^2(G)$ in terms of $n, m, \Delta, \delta, ID(G)$, $IED(G)$, $M_1^2(G)$ and $M_2^1(G)$ respectively. Furthermore, (Refer Table 3- Table 6) we showed that our bounds have the smallest deviation from the first reformulated Zagreb index $EM_1^2(G)$ and superior than the existing bounds in the literature.

2. Preliminaries

As usual $P_n, K_{1,n-1}$ and C_n denote a path, star and a cycle of order *n*, respectively. Let *G* and *H* be graphs. We denote the number of distinct subgraphs of the graph *G* which are isomorphic to *H* by $\sigma_G(H)$. In specific, *G* has $\sigma_G(P_1)$ vertices, $\sigma_G(P_2)$ edges and $\sigma_G(C_3)$ triangles. Let α and β be positive integers, then the double star $D_{\alpha,\beta}$ is a tree on $\alpha+\beta+2$ vertices obtained from the path P_2, by attaching α pendent vertices to its one vertex, and β pendent vertices to its other vertex.

GraphTea [1] is a software tool for graph problems with a focus on extracting information and visualization. It offers powerful ways to query or directly interact with properties of a particular instance of a graph problem. It is specially designed for the computational works on the topological indices.

To analyse and compare our results, we need to recall few classes of graphs:

- The *wheel* W_n is join of the graphs C_{n-1} and K_1.
- The *crown* Cr_n is obtained from the cycle C_n by adjoining a pendant edge at each vertex of the cycle.
- The *helm* H_n is obtained from the wheel graph W_{n-1} by adjoining a pendant edge at each vertex of the cycle.
- The *flower* Fl_n is obtained from the helm H_n by joining each pendent vertex to the central vertex of the helm.
- A graph *G* is called *bidegreed* if its vertex degree is either Δ or δ with $\Delta > \delta \geq 1$.

In 2010, Zhou and Trinajstić [20] obtained the following identity.

Proposition 2.1. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1^2(G) = M_1^3(G) + 2M_2^1(G) - 4M_1^2(G) + 4m. \quad (2.1)$$

Using the results from [4] without exaggeration, we obtain the following corollary for $EM_1^2(G)$ in terms of its subgraphs of *G*.

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

$$EM_1^2(G) = 6\sigma_G(K_{1,3}) + 2\sigma_G(P_4) + 2\sigma_G(P_3) + 6\sigma_G(P_3).$$

3. Lower Bounds on the First Reformulated Zagreb Index

In 2012, Ilić and Zhou [11] proposed the following lower bound for $EM_1^2(G)$.

Lemma 3.1. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1^2(G) \geq \frac{2m}{n} M_1^2(G) + 2M_2^1(G) - 4M_1^2(G) + 4m \quad (3.1)$$

with equality if and only if G is regular.

Very recently in 2016, Milovanović, Dolićanin, Glogić [16] obtained the new lower bounds for $EM_1^2(G)$ in terms of $M_1^2(G)$ and $M_2^1(G)$.

Lemma 3.2. *Let G be a simple graph with* $n(n \geq 2)$ *vertices and m edges. Then*

$$EM_1^2(G) \geq \frac{M_1^2(G)^2}{2m} + 2M_2^1(G) - 4M_1^2(G) + 4m \quad (3.2)$$

$$EM_1^2(G) \geq 4\left(M_2^1(G) - M_1^2(G) + m\right) \quad (3.3)$$

equality holds if and only if G is a regular.

Remark 3.3. *In 2015, Fortula and Gutman* [8] *have given the following lower bounds for* $M_1^3(G)$. *Let G be a graph with m edges. Then*

$$M_1^3(G) \geq \frac{\left(M_1^2(G)\right)^2}{2m} \quad (3.4)$$

$$M_1^3(G) \geq \frac{\left(M_1^2(G)\right)^2}{2m} - 2M_2^1(G). \quad (3.5)$$

Note that, the equality of (3.4) *holds if and only if G is regular. It is easy to see that, the inequality* (3.2) *can be obtained from* (2.1) *by using* (3.4).

In analogy, one can propose a lower bound for $EM_1^2(G)$ using (3.5). But in 2012, De [6] obtained the following inequality.

Lemma 3.4. *Let G be a simple graph with* $n(n \geq 2)$ *vertices and m edges. Then*

$$EM_1^2(G) \geq \frac{\left(M_1^2(G)\right)^2}{m} - 4M_1^2(G) + 4m \quad (3.6)$$

equality holds if and only if G is a regular.

In 2010, Zhou and Trinajstić [19] proposed the following inequality in the context of general sum connectivity.

Lemma 3.5. *Let G be a graph with* $m \geq 1$ *edges. If* $0 < \alpha < 1$, *then* $\chi^\alpha(G) \leq M_1^2(G)^\alpha m^{1-\alpha}$, *and if* $\alpha < 0$ *or* $\alpha > 1$, *then* $\chi^\alpha(G) \geq M_1^2(G)^\alpha m^{1-\alpha}$, *and either equality holds if and only if d(u) + d(v) is a constant for any edge uv.*

Note that, for $\alpha = 2$ in Lemma 3.5 turns (3.5) as its special case. Also from Lemma 3.5, it is clear that the equality of (3.6) holds if and only if *d*(*u*) + *d*(*v*) is a constant for any edge *uv:* In addition, from [8], it is easy to see that (3.2) and (3.6) are incomparable.

Now, we are ready to present our lower bounds on $EM_1^2(G)$ in terms of $n, m, \Delta, \delta, ID(G), M_1^2(G)$ and $M_2^1(G)$.

Theorem 3.6. *Let G be a simple graph with n vertices and m edges, then*

$$EM_1^2(G) \geq \frac{M_1^2(G)^2}{2m} + \frac{1}{2m}\left(2mID(G) - n^2\right) + 2M_2^1(G) - 4M_1^2(G) + 4m \quad (3.7)$$

equality holds if and only if G is regular.

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

$$\sum_{i=1}^{k} w_i a_i^2 \sum_{i=1}^{k} w_i b_i^2 \geq \left(\sum_{i=1}^{k} w_i a_i\, b_i\right)^2. \quad (3.8)$$

Since w_i is non-negative, we assume that $w_i = m_i - n_i$ such that $m_i \geq n_i \geq 0$. Thus

$$\sum_{i=1}^{k} m_i a_i^2 \sum_{i=1}^{k} m_i b_i^2 - \left(\sum_{i=1}^{k} m_i a_i\, b_i\right)^2 \geq \sum_{i=1}^{k} n_i a_i^2 \sum_{i=1}^{k} n_i b_i^2 - \left(\sum_{i=1}^{k} n_i a_i\, b_i\right)^2 \geq 0. \quad (3.9)$$

Set $m_i = d(v_i), n_i = \frac{1}{d(v_i)}, a_i = d(v_i)$ and $b_i = 1,$ for all $i = 1, 2, ..., n$ in the above, we get

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

The inequality (3.7) is obtained from the above inequality and equality (2.1) and the equality holds if and only if G is regular.

Theorem 3.7. *Let G be a simple graph with n vertices and m edges, then*

$$EM_1^2(G) \geq \frac{M_1^2(G)^2}{2m} + \frac{1}{2m}\left(nM_1^2(G) - 4m^2\right) + 2M_2^1(G) - 4M_1^2(G) + 4m \quad (3.10)$$

equality holds if and only if G is regular.

Proof. The proof follows from the same terminology of Theorem 3.6 by choosing $m_i = d(v_i)$, $n_i = 1, a_i = d(v_i)$ and $b_i = 1,$ for all $i = 1, 2, ..., n.$

Remark 3.8. For every simple graph G, the lower bound in (3.10) is always better than the lower bound in (3.7). For this, we have to show that

$$nM_1^2(G) - 4m^2 \geq 2mID(G) - n^2 \geq 0. \quad (3.11)$$

By fixing $a_i = d(v_i), b_i = 1, m_i = 1$ *and* $n_i = d(v_i)^{-1}$ *in* (3.9), *we achieve our required claim and the equality holds if and only if G is regular. Therefore inequality* (3.10) *is stronger than* (3.7) *and* (3.7) *is stronger than* (3.2).

Remark 3.9. *On the other hand, the lower bounds in* (3.6) *and* (3.10) *are incomparable. For Helm* $H_n(n \geq 4)$ *the lower bound in* (3.10) *is better than* (3.6) *and for the Flower* $F_n(n \geq 4)$ *the lower bound in* (3.6) *is better than* (3.10). *In addition for the Crown* Cr_n *both the lower bounds coincides together, other than the equality case.*

Next, we need to improve the lower bound (3.6). For which we need the following inequality which relates the first Zagreb index, second Zagreb index and the forgotten topological index.

Theorem 3.10. *Let G be a simple graph with no isolated edges, then*

$$M_1^3(G) \geq \frac{M_1^2(G)^2}{m} + \frac{1}{m}\left[M_1^2(G) - 2m\right] IED(G) - 2M_2^1(G) - m \quad (3.12)$$

equality holds if and only if d(u) + d(v) is a constant for any edge uv.

Proof. Considering the weighted version of Cauchy-Schwartz inequality from (3.8) with the assumption $w_i = x_i - y_i$ such that $x_i \geq y_i \geq 0$ and by setting $x_i = 1,$ $y_i = \frac{1}{d(e_i)}, a_i = d(e_i)$ and $b_i = 1,$ for all $i = 1, 2, ..., m,$ we get

$$\sum_{i=1}^{m} d(e_i)^2 \sum_{i=1}^{m} 1 - \left(\sum_{i=1}^{m} d(e_i)\right)^2 \geq \sum_{i=1}^{m} d(e_i) \sum_{i=1}^{m} \frac{1}{d(e_i)} - \left(\sum_{i=1}^{m} 1\right)^2$$

expanding, we have

$$\begin{pmatrix} M_1^3(G) + M_2^1(G) \\ +4m - 4M_1^2(G) \end{pmatrix} m - \left(M_1^2(G) - 2m\right)^2 \geq \left(M_1^2(G) - 2m\right) IED(G) - m^2,$$

and the equality holds if and only if $d(u)$ + $d(v)$ is a constant for any edge uv, which completes our claim.

Corollary 3.11. *With the assumptions in Theorem* 3.10, *we have*

$$EM_1^2(G) \geq \frac{M_1^2(G)^2}{m} + \frac{1}{m}\left[M_1^2(G) - 2m\right] IED(G) - 4M_1^2(G) + 3m \quad (3.13)$$

equality holds if and only if d(u) + d(v) is a constant for any edge uv.

Remark 3.12. *Still the lower bound in* (3.10) *and* (3.13) *are incomparable. Consider the Helm* $H_n(n \geq 4)$, *for which the lower bound in* (3.10) *is finer than* (3.13) *and for the complement* $H_n(n \geq 4)$ *the lower bound in* (3.13) *is finer than* (3.10).

Our next interest is to reduce the deviation for the lower bounds from the first reformulated Zagreb index. To achieve our goal, either we need to fit some good lower bounds for M_1^3 or some good upper bounds for $M_1^2(G)$ in the equality (2.1).

In 2011, Ilić and Liu [10] proposed a new upper bound for the first Zagreb index $M_1^2(G)$ and proved that it has the smallest deviation from the first Zagreb index.

Lemma 3.13. *Let G be a simple regular graph with n vertices and m edges, with a vertices of maximum degree* Δ *and b vertices of minimum degree* δ*. Then*

$$M_1^2(G) \le 2m(\Delta+\delta) - n\Delta\delta - (\Delta-\delta-1)(n-a-b), \quad (3.14)$$

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

Thus we can state the following result.

Corollary 3.14. *With the assumptions in Lemma 3.13, we have*

$$EM_1^2(G) \ge M_1^3(G) + 2M_2^1(G) - 8m(\Delta+\delta) + 4n\Delta\delta + 4(\Delta-\delta-1)(n-a-b) + 4m, \quad (3.15)$$

To the best knowledge of the authors, still now in the literature (3.14) is superior upper bound for the first Zagreb index $M_1^2(G)$. This motivates us to present the new upper bound which is stronger than (3.14) and which leads to be the better lower bound for the first reformulated Zagreb index $EM_1^2(G)$.

Theorem 3.15. *Let G be a simple graph with n non-isolated vertices and m edges, with a vertices of maximum degree* Δ *and b vertices of minimum degree* δ*. Then*

$$M_1^2(G) \le a\Delta^2 + b\delta^2 + (2m - a\Delta - b\delta)(\Delta+\delta+1) + (\Delta-1)(\delta+1)\left[ID(G) - \frac{a}{\Delta} - \frac{b}{\delta}\right] - (\Delta\delta - 2\Delta - 1)(n-a-b), \quad (3.16)$$

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

Proof. Let $a, A \in \mathbb{R}$ and x_i, y_i be two sequences with the property $ay_i \le x_i \le Ay_i$ for $i = 1, 2, \dots, n$ and w_i be any sequence of positive real numbers, it holds

$$w_i(Ay_i - x_i)(x_i - ay_i) \ge 0. \quad (3.17)$$

Since w_i is a positive sequence, choose $w_i = m_i - n_i$ such that $m_i \ge n_i$ and by setting $A = \Delta$, $a = \delta$, $x_i = d(v_i)$, $y_i = 1$, $m_i = 1$ and $n_i = \frac{1}{d(v_i)}$ and adding over the vertices by restricting $\delta < d(v_i) < \Delta$, we have

$$\sum_{\delta<d(v_i)<\Delta} \left(1 - \frac{1}{d(v_i)}\right)(\Delta - d(v_i))(d(v_i) - \delta) \ge \sum_{\delta<d(v_i)<\Delta} \left(1 - \frac{1}{d(v_i)}\right)(\Delta-\delta-1) \ge 0, \quad (3.17)$$

expanding the above inequality gives the required result with equality if and only if $d(v_i) = \delta+1$ or $d(v_i) = \Delta-1$. This completes the proof.

The computational results for connected graphs on n = 3 to 9 vertices and connected trees on n = 10 to 20 vertices are provided in Table 1 and Table 2 respectively.

Table 1. Upper bound comparision of $M_1^2(G)$ for small graphs

Parameters			Parameters			Lemma 3.13		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	9.0000	9.0000	0.0000	2	9.0000	0.0000	2
4	6	19.6667	19.6667	0.0000	6	19.6667	0.0000	6
5	21	35.4286	35.4286	0.0000	21	35.4286	0.0000	21
6	112	55.6607	55.7440	0.3883	106	55.7857	0.5825	106
7	853	82.6260	83.0240	1.1093	683	83.1981	1.5869	683
8	11117	118.4507	119.6036	2.4343	6658	120.0452	3.3453	6658
9	261080	166.1056	168.6350	4.5110	105659	169.4830	5.9966	105659

Table 2. Upper bound comparison of $M_1^2(G)$ for small trees

Parameters			Parameters			Lemma 3.13		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	44.5849	44.7311	0.4200	91	44.8019	0.6219	91
11	235	50.0255	50.2645	0.6064	189	50.3787	0.8921	189
12	551	55.4011	55.7551	0.8162	413	55.9220	1.1936	413
13	1301	60.7640	61.2498	1.0509	913	61.4766	1.5299	913
14	3159	66.1292	66.7626	1.3027	2075	67.0560	1.8898	2075
15	7741	71.4949	72.2915	1.5748	4774	72.6583	2.2783	4774
16	19320	76.8598	77.8323	1.8611	11214	78.2780	2.6862	11214
17	48629	82.2303	83.3931	2.1644	26619	83.9238	3.1180	26619
18	123867	87.6032	88.9683	2.4803	64057	89.5893	3.5673	64057
19	317955	92.9794	94.5599	2.8104	155575	95.2768	4.0365	155575
20	823065	98.3585	100.1660	3.1522	381521	100.9836	4.5219	381521

In the group one of the Table 1 and Table 2, the first column represents the degree of the vertex n, the second column contains number of connected graphs (trees) on n vertices and the third one has the average value of the first Zagreb index $M_1^2(G)$. Next two groups of three columns represent the average value of the upper bound, the standard deviation

$$\left(\sqrt{\frac{\sum_G\left(X(G)-M_1^2(G)\right)^2}{count}}\right)$$

and the number of graphs with equality case.

On comparison of the computational results in Table 1 and Table 2, we observe it is coherent that the upper bound (3.16) has the least deviation from $M_1^2(G)$ and stronger than (3.14).

Corollary 3.16. *With the assumptions in Theorem 3.15, we have*

$$\begin{aligned}EM_1^2(G) \geq\ & M_1^3(G)+2M_2^1(G) \\ & +4(\Delta-\delta-1)(n-a-b)+4m \\ & -4(\Delta-1)(\delta+1)\left[ID(G)-\frac{a}{\Delta}-\frac{b}{\delta}\right] \\ & -4\left(a\Delta^2+b\delta^2\right) \\ & -4(2m-a\Delta-b\delta)(\Delta+\delta+1)\end{aligned} \quad (3.18)$$

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

In analogy, Table 3 - Table 4 conclude that the lower bound (3.18) has the least deviation from $M_1^2(G)$ and so it is superior than the existing lower bounds.

Table 3. Lower bound comparison of $EM_1^2(G)$ for small graphs

Parameters			Corollary 3.16			Corollary 3.14		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	7.0000	7.0000	0.0000	2	7.0000	0.0000	2
4	6	34.6667	34.6667	0.0000	6	34.6667	0.0000	6
5	21	96.2857	96.2857	0.0000	21	96.2857	0.0000	21
6	112	195.9643	195.6310	1.5533	106	195.4643	2.3299	106
7	853	356.3329	354.7409	4.4371	683	354.0445	6.3475	683
8	11117	605.4936	600.8817	9.7374	6658	599.1156	13.3811	6658
9	261080	991.0099	980.8922	18.0439	105659	977.5002	23.9863	105659
Parameters			Theorem 3.7			Corollary 3.11		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	7.0000	6.7500	0.3536	1	7.0000	0.0000	2
4	6	34.6667	33.1389	2.1093	2	34.3500	0.4732	3
5	21	96.2857	91.2316	6.4066	2	94.3278	2.3736	4
6	112	195.9643	185.4258	13.0763	5	190.4460	6.3778	7
7	853	356.3329	336.8463	23.2882	4	344.2109	13.6459	7
8	11117	605.4936	573.8401	36.7729	17	583.5165	24.4070	20
9	261080	991.0099	942.5787	54.9013	22	954.9776	39.5418	27

Table 4. Lower bound comparison of $EM_1^2(G)$ for small trees

Parameters			Corollary 3.16			Corollary 3.14		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	99.4151	98.8302	1.6798	91	98.5472	2.4877	91
11	235	114.4340	113.4780	2.4256	189	113.0213	3.5682	189
12	551	128.7477	127.3316	3.2649	413	126.6642	4.7744	413
13	1301	142.8932	140.9500	4.2035	913	140.0430	6.1195	913
14	3159	156.9839	154.4501	5.2108	2075	153.2764	7.5592	2075
15	7741	171.0559	167.8697	6.2993	4774	166.4023	9.1131	4774
16	19320	185.1062	181.2163	7.4443	11214	179.4335	10.7449	11214
17	48629	199.2024	194.5513	8.6574	26619	192.4283	12.4720	26619
18	123867	213.3222	207.8617	9.9211	64057	205.3778	14.2694	64057
19	317955	227.4755	221.1534	11.2414	155575	218.2861	16.1458	155575
20	823065	241.6596	234.4294	12.6088	381521	231.1590	18.0876	381521
Parameters			Theorem 3.7			Corollary 3.11		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	99.4151	71.2432	45.7847	0	88.7336	13.3439	1
11	235	114.4340	82.1421	52.2828	0	101.0084	17.0481	1
12	551	128.7477	92.8494	57.5453	0	112.6745	20.6571	1
13	1301	142.8932	103.3729	62.4065	0	124.1590	24.3165	1
14	3159	156.9839	113.9656	66.7328	0	135.6441	27.8509	1
15	7741	171.0559	124.5123	70.8548	0	147.1143	31.3411	1
16	19320	185.1062	135.0994	74.7407	0	158.6074	34.7026	1
17	48629	199.2024	145.7020	78.5596	0	170.1444	38.0023	1
18	123867	213.3222	156.3424	82.3052	0	181.7243	41.2101	1
19	317955	227.4755	167.0016	86.0265	0	193.3383	44.3579	1
20	823065	241.6596	177.6906	89.7288	0	204.9893	47.4428	1

4. Upper Bounds on the First Reformulated Zagreb Index

In 2010, Zhou and Trinajstić [20] proposed the first upper bound for $EM_1^2(G)$.

Lemma 4.1. *Let G be a graph on n vertices and* $m \ge 1$ *edges. Then*

$$EM_1^2(G) \le (n-4)M_1^2(G) + 4M_2^1(G) - 4m^2 + 4m \quad (4.1)$$

equality holds if and only if any two non-adjacent vertices have equal degrees.

In 2012, Ilić and Zhou [11] obtained the following upper bound for $EM_1^2(G)$.

Lemma 4.2. *Let G be a simple graph with n vertices and m edges. Then*

$$\begin{aligned} EM_1^2(G) &\le (\Delta+\delta-4)M_1^2(G) \\ &+ 2M_2^1(G) - 2m\Delta\delta + 4m \end{aligned} \quad (4.2)$$

equality holds if and only if G is a regular or bidegreed graph.

In the same time period, De [6] Proposed the following upper bounds for $EM_1^2(G)$.

Lemma 4.3. *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1^2(G) \le 2(\Delta+\delta-2)M_1^2(G) - 4m(\Delta\delta-1) \quad (4.3)$$

$$\begin{aligned} EM_1^2(G) &\le \left(M_1^2(G) - 2m\right)\left(m + 2\delta - 3\right) \\ &- 2m(m-1)(\delta-1) \end{aligned} \quad (4.4)$$

equality holds if and only if G is regular.

In 2016, Milovanović et. al. [16] obtained some new upper bounds for the first reformulated Zagreb index.

Lemma 4.4. *Let G be a simple graph with* $n(n \ge 2)$ *vertices and m edges. Then*

$$\begin{aligned} EM_1^2(G) &\le \frac{M_1^2(G)^2}{2m} + 2M_2^1(G) \\ &- 4M_1^2(G) + \frac{m}{2}(\Delta-\delta)^2 + 4m \end{aligned} \quad (4.5)$$

equality holds if and only if G is regular or $G \cong K_{1,n-1}$. *Moreover,*

$$EM_1^2(G) \le \frac{\left(M_1^2(G) - 2m\right)^2}{m} + m(\Delta-\delta)^2 \quad (4.6)$$

$$EM_1^2(G) \le \frac{\left(M_1^2(G) - 2m\right)^2}{m} + 2m\left(M_1^2(G) - \frac{4m^2}{n}\right) \quad (4.7)$$

equality holds if and only if G is regular.

Remark 4.5. *The upper bounds in* (4.2) *and* (4.3) *are emerged from Diaz-metcalf inequality, by considering the vertex and edge degrees respectively. At first, it is easy to see that the bounds in* (4.1) *and* (4.2) *are always better than* (4.3) *and* (4.4). *Secondly, the upper bound* (4.2) *is always better than the upper bounds* (4.5), (4.6) *and* (4.7), *so we leave it to the fascinated reader. In addition, the bounds in* (4.1) *and* (4.2) *are incomparable. For Helm Graphs* H_n, (4.2) *is better than* (4.1), *and for the Flower graphs* F_n, (4.1) *is better than* (4.2).

Next, we are ready to present our inequality that determines upper bound for the forgotten topological index $M_1^3(G)$ in terms of $n, m, \Delta, M_1^2(G)$, and $M_2^1(G)$, which leads to the upper bound for $EM_1^2(G)$.

Theorem 4.6. *Let G be a simple graph with n non-isolated vertices and m edges, with a vertices of maximum degree* Δ *and b vertices of minimum degree* δ. *Then*

$$\begin{aligned} M_1^3(G) &\le a\Delta^3 + b\delta^3 + (\Delta+\delta)\begin{pmatrix} M_1^2(G) - a\left(\Delta^2+1\right) \\ -b\left(\delta^2+1\right) - n \end{pmatrix} \\ &+ (\Delta-1)(\delta+1)\left[ID(G) - \frac{a}{\Delta} - \frac{b}{\delta}\right] \\ &- \left((\Delta-1)(\delta+1)-1\right)\left(2m - a\Delta - b\delta\right) \end{aligned} \quad (4.8)$$

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

Proof. The proof follows the same terminology of Theorem 3.15, by the choice of setting $m_i = d(v_i)$ and $n_i = \dfrac{1}{d(v_i)}$.

Corollary 4.7. *With the assumptions in Theorem 4.6, we have*

$$\begin{aligned} &EM_1^2(G) \\ &\le a\Delta^3 + b\delta^3 + (\Delta-1)(\delta+1)\left[ID(G) - \frac{a}{\Delta} - \frac{b}{\delta}\right] \\ &+ (\Delta-\delta)\left(M_1^2(G) - a\left(\Delta^2+1\right) - b\left(\delta^2+1\right) - n\right) \\ &+ 2M_2^1(G) - \left((\Delta-1)(\delta+1)-1\right)\left(2m - a\Delta - b\delta\right) \\ &- 4M_1^2(G) + 4m \end{aligned} \quad (4.9)$$

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

Corollary 4.8. *Let G be a simple graph with n vertices and m edges, with a vertices of maximum degree* Δ *and b vertices of minimum degree* δ. *Then*

$$\begin{aligned} &EM_1^2(G) \\ &\le a\Delta^3 + b\delta^3 + (\Delta+\delta+1)\left(M_1^2(G) - a\Delta^2 - b\delta^2\right) \\ &+ (\Delta-1)(\delta+1)(n-a-b) \\ &- (\Delta\delta + 2\Delta - 1)(2m - a\Delta - b\delta) \\ &+ 2M_2^1(G) - 4M_1^2(G) + 4m \end{aligned} \quad (4.10)$$

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

Proof. The proof follows the same terminology of Theorem 3.15, by the choice of setting $m_i = d(v_i)$ and $n_i = 1$ and using the equality (2.1).

From Table 5-Table 6 (with same notations in Table 1-Table 2), our upper bound (4.10) has the small deviation from $M_1^2(G)$ which concludes that (4.10) is the superior than the existing upper bounds.

We end the paper by remarking that the lower and upper bounds of $EM_1^2(G)$ is determined in terms of *n; m;* $ID(G), M_1^2(G)$ and $M_2^1(G)$. In addition, we presented the upper bound for the first Zagreb index $M_1^2(G)$ and the forgotten topological index $M_1^3(G)$ and with the assistance of computational results, we conclude that these inequalities are superior than the other bounds appeared in the literature so far.

Table 5. Upper bound comparison of $EM_1^2(G)$ for small graphs

Parameters			Corollary 4.8			Corollary 4.7		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	7.0000	7.0000	0.0000	2	7.0000	0.0000	2
4	6	34.6667	34.6667	0.0000	6	34.6667	0.0000	6
5	21	96.2857	96.2857	0.0000	21	96.2857	0.0000	21
6	112	195.9643	196.2143	1.1650	106	196.2976	1.5533	106
7	853	356.3329	357.6764	3.8272	683	358.0744	4.9305	683
8	11117	605.4936	609.8366	9.4456	6658	610.9895	11.8628	6658
9	261080	991.0099	1001.5845	19.3717	105659	1004.1139	23.8496	105659
Parameters			Lemma 4.1			Lemma 4.2		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
3	2	7.0000	7.0000	0.0000	2	7.0000	0.0000	2
4	6	34.6667	35.3333	1.6330	5	35.3333	1.1547	4
5	21	96.2857	99.6190	5.9362	11	99.6190	4.9570	8
6	112	195.9643	205.9107	15.0772	36	206.0000	13.0767	15
7	853	356.3329	380.2673	31.8992	91	378.1290	26.5012	25
8	11117	605.4936	652.0770	58.6369	471	644.4005	45.5048	53
9	261080	991.0099	1072.0948	98.1035	2296	1052.3611	70.0854	95

Table 6. Upper bound comparison of $EM_1^2(G)$ for small trees

Parameters			Corollary 4.8			Corollary 4.7		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	99.4151	99.8679	1.3175	91	100.0142	1.7358	91
11	235	114.4340	115.1830	1.9439	189	115.4220	2.5469	189
12	551	128.7477	129.8730	2.6727	413	130.2270	3.4831	413
13	1301	142.8932	144.4520	3.4937	913	144.9377	4.5362	913
14	3159	156.9839	159.0326	4.3828	2075	159.6660	5.6745	2075
15	7741	171.0559	173.6478	5.3461	4774	174.4444	6.9074	4774
16	19320	185.1062	188.2864	6.3635	11214	189.2589	8.2089	11214
17	48629	199.2024	203.0205	7.4434	26619	204.1833	9.5900	26619
18	123867	213.3222	217.8203	8.5705	64057	219.1854	11.0310	64057
19	317955	227.4755	232.6989	9.7500	155575	234.2795	12.5388	155575
20	823065	241.6596	247.6490	10.9734	381521	249.4566	14.1024	381521
Parameters			Lemma 4.1			Lemma 4.2		
n	Count	Avg.	Avg.	Stdev.	Eq.	Avg.	Stdev.	Eq.
10	106	99.4151	113.8491	16.2724	5	164.3774	68.8660	1
11	235	114.4340	133.5319	21.2783	3	201.2426	91.8521	1
12	551	128.7477	152.3194	26.3422	5	240.4646	118.3697	1
13	1301	142.8932	171.5634	31.9734	2	282.1168	147.5565	1
14	3159	156.9839	190.7692	37.7317	10	326.6477	179.9576	1
15	7741	171.0559	210.3741	43.8713	2	373.8465	215.0847	1
16	19320	185.1062	230.0205	50.1354	9	423.8166	253.1651	1
17	48629	199.2024	249.9992	56.6729	6	476.5955	294.0235	1
18	123867	213.3222	270.1175	63.3533	16	532.1868	337.7529	1
19	317955	227.4755	290.4733	70.2383	2	590.5895	384.2730	1
20	823065	241.6596	310.9927	77.2696	27	651.8210	433.6323	1

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