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Some Properties of the Zagreb Indices

Emina Milovanović[a], Igor Milovanović[a], Muhammad Jamil[b]

[a]*Faculty of Electronics Engineering, University of Niš, A. Medvedeva 14, 18000 Niš, Serbia*
[b]*Department of mathematics, Riphah institute of computing and applied sciences, Riphah international university, Lahore, Pakistan.*

Abstract. Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, $E = \{e_1, e_2, \ldots, e_m\}$, be a simple graph with n vertices and m edges. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$, sequences of vertex and edge degrees, respectively. If i-th and j-th vertices of G are adjacent, it is denoted as $i \sim j$. Graph invariants referred to as the first, second and the first reformulated Zagreb indices are defined as $M_1 = \sum_{i=1}^{n} d_i^2$, $M_2 = \sum_{i\sim j} d_i d_j$ and $EM_1 = \sum_{i=1}^{m} d(e_i)^2$, respectively. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be eigenvalues of G. With $\rho(G) = \lambda_1$ a spectral radius of G is denoted. Lower bounds for invariants M_1, M_2, EM_1 and $\rho(G)$ are obtained.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, $E = \{e_1, e_2, \ldots, e_m\}$, be a simple graph, with the sequence of vertex degrees $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $d_i = d(i)$ $(i = 1, 2, \ldots, n)$ and the sequence of edge degrees $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m) > 0$. If i-th and j-th vertices (edges) of the graph G are adjacent, we denote it as $i \sim j$ $(e_i \sim e_j)$. The edge connecting vertices i and j will be denoted by $e = \{i, j\}$. The degree of edge $e = \{i, j\}$ is defined as $d(e) = d_i + d_j - 2$.

A single number that can be used to characterize some property of the graph is called a *topological index* for that graph. Obviously, the number of vertices and the number of edges are topological indices.

Two vertex-degree based topological indices, the first and the second Zagreb index, M_1 and M_2, are defined as (see [12])

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \qquad \text{and} \qquad M_2 = M_2(G) = \sum_{i\sim j} d_i d_j.$$

The Zagreb indices are among the oldest and most studied molecular structure descriptors and found significant applications in chemistry. Nowadays, there exist hundreds of papers on Zagreb indices and related matter. For the recent results on Zagreb indices, the interested reader can refer to [1, 9, 10, 13, 18, 22, 30, 33]. Let us note that the Zagreb indices are special cases of Randić index (see for example [20, 21, 28]). Details on other vertex–based topological indices can be found in [11, 27].

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Email addresses: ema@elfak.ni.ac.rs (Emina Milovanović), igor@elfak.ni.ac.rs (Igor Milovanović), m.kamran.sms@gmail.com (Muhammad Jamil)

In [24], an edge-degree graph topological index, named reformulated first Zagreb index, EM_1, is defined as

$$EM_1 = EM_1(G) = \sum_{i=1}^{m} d(e_i)^2 = \sum_{e_i \sim e_j} (d(e_i) + d(e_j)).$$

Denote by **A** the adjacency matrix of G. The eigenvalues of adjacency matrix **A**, $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, represent ordinary eigenvalues of the graph G. The eigenvalue $\lambda_1 = \rho(G)$ is referred to as spectral radius of graph G (see for example [2, 32, 34]).

The first and reformulated first Zagreb indices, particulary theirs upper/lower bounds has attracted recently the attention of many mathematicians and computer scientists (see for example [6, 8, 15–17, 24, 25, 29, 35]). In this paper we state some new inequalities that set lower bounds for the invariants M_1 and EM_1. Some of the obtained inequalities are generalization of the results published in the literature. As a corollaries of the obtained results, lower bounds of graph invariants M_2 and $\lambda_1 = \rho(G)$ are acquired.

2. Preliminaries

In what follows, we outline a few results of spectral graph theory that will be needed in the subsequent considerations.

The following lower bounds of M_1 and M_2 in terms of parameters n, m, d_1, d_2 and d_n were obtained in [5]:

Lemma 2.1. [5] *Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_1 \geq d_1^2 + \frac{(2m-d_1)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(d_2-d_n)^2. \tag{1}$$

Equality holds if and only if G is regular graph or with the property $d_2 = d_3 = \cdots = d_n$.

Lemma 2.2. [5] *Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_2 \geq 2m^2 - (n-1)md_1 + \frac{1}{2}(d_1-1)\left(d_1^2 + \frac{(2m-d_1)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(d_2-d_n)^2\right), \tag{2}$$

with equality if and only if G is regular.

In [4] (see also [5]) the following inequality was proved.

Lemma 2.3. [4] *Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_2 \geq 2m^2 - (n-1)md_1 + \frac{1}{2}(d_1-1)M_1 \tag{3}$$

with equality if and only if G is regular.

In [3] the following result that determines the lower bound of M_1 in terms of m, n, d_1 and d_n was proved.

Lemma 2.4. [3] *Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_1 \geq d_1^2 + d_n^2 + \frac{(2m-d_1-d_n)^2}{n-2}, \tag{4}$$

with equality if and only if G is regular or with the property $d_2 = d_3 = \cdots = d_{n-1}$.

In [7] (see also [15, 19, 31] the lower bound of M_1 in terms of n and m was determined.

Lemma 2.5. [7] *Let G be a simple connected graph with n vertices and m edges. Then*

$$M_1 \geq \frac{4m^2}{n}. \tag{5}$$

Equality holds if and only if G is regular.

The following lower bound of the spectral radius of graph, $\lambda_1 = \rho(G)$, in terms of parameters n and m was determined in [2]:

Lemma 2.6. [2] *Let G be a simple connected graph with n vertices and m edges. Then*

$$\lambda_1 = \rho(G) \geq \frac{2m}{n}. \tag{6}$$

Equality holds if and only if G is regular.

In [16] (see also [6]) the following lower bound for the invariant EM_1 in terms of M_1 and m was determined:

Lemma 2.7. [16] *Let G be a simple graph with n vertices and $m \geq 1$ edges. Then*

$$EM_1 \geq \frac{(M_1 - 2m)^2}{m}. \tag{7}$$

Equality holds if and only if G is regular.

3. Main results

In the following theorem we prove the inequality that determines the lower bound for M_1 which is better than (5).

Theorem 3.1. *Let G be a simple graph of order n ($n \geq 2$) with m edges and without isolated vertices. Let k_1 and k_2 be arbitrary real numbers with the properties $d_1 \geq k_1 \geq \frac{2m}{n}$ and $\frac{2m}{n} \geq k_2 \geq d_n$. Then*

$$M_1 \geq \frac{4m^2}{n} + \alpha(k_1, k_2), \tag{8}$$

where

$$\alpha(k_1, k_2) = \max\left\{\frac{(nk_1 - 2m)^2}{n(n-1)}, \frac{(2m - nk_2)^2}{n(n-1)}, \frac{1}{2}(d_1 - d_n)^2\right\}.$$

Equality holds if and only if G is a regular graph.

Proof. In [23] a class of real polynomials $\mathcal{P}_n(a_1, a_2)$ of the form $P_n(x) = x^n + a_1x^{n-1} + a_2x^{n-2} + b_3x^{n-3} + \cdots + b_n$, where a_1 and a_2 are fixed real numbers, was considered. Let $x_1 \geq x_2 \geq \cdots \geq x_n$ be real roots of the polynomial $P_n(x) \in \mathcal{P}_n(a_1, a_2)$. Then

$$\bar{x} + \frac{1}{n}\sqrt{\frac{\Delta}{n-1}} \leq x_1 \leq \bar{x} + \frac{1}{n}\sqrt{(n-1)\Delta}, \tag{9}$$

$$\bar{x} - \frac{1}{n}\sqrt{\frac{(i-1)\Delta}{n-i+1}} \leq x_i \leq \bar{x} + \frac{1}{n}\sqrt{\frac{(n-i)\Delta}{i}}, \quad i = 2, 3, \ldots, n-1,$$

$$\bar{x} - \frac{1}{n}\sqrt{(n-1)\Delta} \leq x_n \leq \bar{x} - \frac{1}{n}\sqrt{\frac{\Delta}{n-1}}, \tag{10}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \quad \text{and} \quad \Delta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2. \tag{11}$$

Now consider the polynomial

$$P_n(x) = \prod_{i=1}^{n}(x - d_i) = x^n + a_1x^{n-1} + a_2x^{n-2} + b_3x^{n-3} + \cdots + b_n,$$

where $d_1 \geq d_2 \geq \cdots \geq d_n$ are vertex degrees in G. Since

$$a_1 = -\sum_{i=1}^{n} d_i = -2m, \quad a_2 = \frac{1}{2}\left(\left(\sum_{i=1}^{n} d_i\right)^2 - \sum_{i=1}^{n} d_i^2\right) = \frac{1}{2}(4m^2 - M_1),$$

the polynomial $P_n(x)$ belongs to a class of real polynomials $\mathcal{P}_n(-2m, \frac{1}{2}(4m^2 - M_1))$. According to (11) we have that

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} d_i = \frac{2m}{n} \quad \text{and} \quad \Delta = n\sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} d_i\right)^2 = nM_1 - 4m^2. \tag{12}$$

For $x_1 = d_1$ from (12) and the right part of the inequality (9), we have that for each real k_1, $d_1 \geq k_1 \geq \frac{2m}{n}$, holds

$$k_1 \leq d_1 \leq \frac{2m}{n} + \frac{1}{n}\sqrt{(n-1)(nM_1 - 4m^2)},$$

i.e.

$$0 \leq nk_1 - 2m \leq \sqrt{(n-1)(nM_1 - 4m^2)},$$

wherefrom follows

$$M_1 \geq \frac{4m^2}{n} + \frac{(nk_1 - 2m)^2}{n(n-1)}. \tag{13}$$

For $x_n = d_n$, from (12) and left part of the inequality (10), for each k_2, $\frac{2m}{n} \geq k_2 \geq d_n$, holds

$$\frac{2m}{n} - \frac{1}{n}\sqrt{(n-1)(nM_1 - 4m^2)} \leq d_n \leq k_2,$$

i.e.

$$0 \leq 2m - nk_2 \leq \sqrt{(n-1)(nM_1 - 4m^2)},$$

wherefrom follows

$$M_1 \geq \frac{4m^2}{n} + \frac{(2m - nk_2)^2}{n(n-1)}. \tag{14}$$

In [26] the following inequality was proved

$$M_1 \geq \frac{4m^2}{n} + \frac{1}{2}(d_1 - d_n)^2. \tag{15}$$

According to (13), (14) and (15) we obtain (8). □

Remark 3.2. *The inequalities (13), (14) and (15) are stronger than (5). Consequently, (8) is also stronger than (5).*

Corollary 3.3. *Let G be a simple graph of order n ($n \geq 2$) with m edges, without isolated vertices. Then*

$$M_1 \geq \frac{4m^2}{n} + \alpha(d_1, d_n), \tag{16}$$

where

$$\alpha(d_1, d_n) = \max\left\{\frac{(nd_1 - 2m)^2}{n(n-1)}, \frac{(2m - nd_n)^2}{n(n-1)}, \frac{1}{2}(d_1 - d_n)^2\right\}.$$

Equality holds if and only if G is regular.

Proof. The required result is obtained from (8) for $k_1 = d_1$ and $k_2 = d_n$. □

Remark 3.4. *Let us note that values $\frac{(nd_1-2m)^2}{n(n-1)}$, $\frac{(2m-nd_n)^2}{n(n-1)}$ and $\frac{1}{2}(d_1 - d_n)^2$ are incomparable. Thus, for example, if $G = K_{1,n-1}$ then $\frac{(nd_1-2m)^2}{n(n-1)}$ has a maximal value, if $G = P_n$ then $\frac{(2m-nd_n)^2}{n(n-1)}$ is the maximum, and if sequence of vertex degrees of G is of the form $(3, \underbrace{2, \ldots, 2}_{(n-2)-times}, 1)$ then $\frac{1}{2}(d_1 - d_n)^2$ has a maximal value.*

Corollary 3.5. *Let G be a simple connected graph with n vertices and m edges. Then*

$$\lambda_1 \geq \sqrt{\frac{4m^2}{n^2} + \frac{\alpha(d_1, d_n)}{n}}. \tag{17}$$

Equality holds if and only if G is regular.

Proof. The inequality (17) can be obtained from the inequality (16) and inequality $\lambda_1 \geq \sqrt{\frac{M_1}{n}}$ proved in [14]. □

Remark 3.6. *Since $\alpha(d_1, d_n) \geq 0$, the inequality (17) is stronger than (6).*

Corollary 3.7. *Let G be a simple graph with n ($n \geq 3$) vertices and m edges. Then*

$$M_2 \geq 2m^2 - (n-1)md_1 + \frac{1}{2}(d_1 - 1)\left(\frac{4m^2}{n} + \alpha(k_1, k_2)\right). \tag{18}$$

Equality holds if and only if G is regular.

In the following theorem we determine the lower bound of the invariant M_1 in terms of parameters n, m, d_1, d_2 and d_n.

Theorem 3.8. *Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_1 \geq d_1^2 + \frac{(2m - d_1)^2}{n-1} + \frac{1}{2}(d_2 - d_n)^2. \tag{19}$$

Equality holds if and only if G is a regular graph or with the property $d_3 = \cdots = d_{n-1} = \frac{d_2+d_n}{2}$.

Proof. Based on the inequality

$$\begin{aligned}(n-1)\sum_{i=2}^{n} d_i^2 - \left(\sum_{i=2}^{n} d_i\right)^2 &= \sum_{2\leq i<j\leq n} (d_i - d_j)^2 \geq \sum_{i=3}^{n-1}((d_2 - d_i)^2 + (d_i - d_n)^2) + (d_2 - d_n)^2 \\ &\geq \sum_{i=3}^{n-1} \frac{1}{2}(d_2 - d_n)^2 + (d_2 - d_n)^2 = \frac{(n-1)}{2}(d_2 - d_n)^2,\end{aligned}$$

we have that

$$(n-1)(M_1-d_1^2)-(2m-d_1)^2 \geq \frac{(n-1)}{2}(d_2-d_n)^2,$$

wherefrom we obtain (19). □

Corollary 3.9. *Let G be a simple graph with n $(n \geq 3)$ vertices and m edges. Then*

$$M_2 \geq 2m^2-(n-1)md_1+\frac{1}{2}(d_1-1)\left(d_1^2+\frac{(2m-d_1)^2}{n-1}+\frac{1}{2}(d_2-d_n)^2\right). \tag{20}$$

Equality holds if and only if G is regular.

Remark 3.10. *Since for each $n \geq 3$ holds*

$$\frac{1}{2}(d_2-d_n)^2 \geq \frac{2(n-2)}{(n-1)^2}(d_2-d_n)^2$$

it follows that the inequality (19) is stronger than (1), while (20) is stronger than (2).

Corollary 3.11. *Let G be a simple graph with n $(n \geq 3)$ vertices and m edges. Then*

$$\lambda_1=\rho(G) \geq \sqrt{\frac{1}{n}\left(d_1^2+\frac{(2m-d_1)^2}{n-1}+\frac{1}{2}(d_2-d_n)^2\right)}.$$

Equality holds if and only if G is regular.

By the similar procedure as the one applied in the proof of Theorem 3.8, the following result can be proved.

Theorem 3.12. *Let G be a simple graph with n $(n \geq 3)$ vertices and m edges. Then*

$$M_1 \geq d_1^2+d_n^2+\frac{(2m-d_1-d_n)^2}{n-2}+\frac{1}{2}(d_2-d_{n-1})^2. \tag{21}$$

Equality holds if and only if G is a regular graph or with the property $d_3=\cdots=d_{n-2}=\frac{d_2+d_{n-1}}{2}$.

Remark 3.13. *The inequality (21) is stronger than (4).*

Corollary 3.14. *Let G be a simple graph with n $(n \geq 3)$ vertices and m edges. Then*

$$M_2 \geq 2m^2-(n-1)md_1+\frac{1}{2}(d_1-1)\left(d_1^2+d_n^2+\frac{(2m-d_1-d_n)^2}{n-2}+\frac{1}{2}(d_2-d_{n-1})^2\right).$$

Equality holds if and only if G is regular.

In the next theorem we set up the lower bound for the invariant EM_1.

Theorem 3.15. *Let G be a simple graph with n $(n \geq 2)$ vertices and m edges. Let k_3 and k_4 be arbitrary real numbers with the properties*

$$d(e_1) \geq k_3 \geq \frac{M_1-2m}{m} \quad \text{and} \quad \frac{M_1-2m}{m} \geq k_4 \geq d(e_m).$$

Then

$$EM_1 \geq \frac{(M_1-2m)^2}{m}+\alpha(k_3,k_4), \tag{22}$$

where

$$\alpha(k_3,k_4)=\max\left\{\frac{(mk_3-M_1+2m)^2}{m(m-1)}, \frac{(M_1-2m-mk_4)^2}{m(m-1)}, \frac{1}{2}(d(e_1)-d(e_m))^2\right\}.$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. Consider the polynomial

$$P_m(x) = \prod_{i=1}^{m}(x - d(e_i)) = x^m + a_1x^{m-1} + a_2x^{m-2} + b_3x^{m-3} + \cdots + b_m,$$

where $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m) \geq 0$ are edge degrees of G. Since

$$a_1 = -\sum_{i=1}^{m} d(e_i) = -(M_1 - 2m)$$

and

$$a_2 = \frac{1}{2}\left(\left(\sum_{i=1}^{m} d(e_i)\right)^2 - \sum_{i=1}^{m} d(e_i)^2\right) = \frac{1}{2}((M_1 - 2m)^2 - EM_1),$$

the polynomial $P_m(x)$ belongs to a class of polynomials $\mathcal{P}_m(2m - M_1, \frac{1}{2}((M_1 - 2m)^2 - EM_1))$. According to (11) we have that

$$\begin{aligned} \bar{x} &= \frac{1}{m}\sum_{i=1}^{m} d(e_i) = \frac{M_1 - 2m}{m}, \\ \Delta &= m\sum_{i=1}^{m} d(e_i)^2 - \left(\sum_{i=1}^{m} d(e_i)\right)^2 = mEM_1 - (M_1 - 2m)^2. \end{aligned} \tag{23}$$

For $x_1 = d(e_1)$, from (23) and right part of the inequality (9), for each real k_3, $d(e_1) \geq k_3 \geq \frac{M_1-2m}{m}$, we have that

$$k_3 \leq d(e_1) \leq \frac{M_1 - 2m}{m} + \frac{1}{m}\sqrt{(m-1)(mEM_1 - (M_1 - 2m)^2)},$$

i.e.

$$0 \leq mk_3 - M_1 + 2m \leq \sqrt{(m-1)(mEM_1 - (M_1 - 2m)^2)},$$

wherefrom it follows that

$$EM_1 \geq \frac{(M_1 - 2m)^2}{m} + \frac{(mk_3 - M_1 + 2m)^2}{m(m-1)}. \tag{24}$$

For $n = m$, $x_m = d(e_m)$, according to (23) and left part of the inequality (10), for each k_4, $\frac{M_1-2m}{m} \geq k_4 \geq d(e_m)$, we have that

$$\frac{M_1 - 2m}{m} - \frac{1}{m}\sqrt{(m-1)(mEM_1 - (M_1 - 2m)^2)} \leq d(e_m) \leq k_4,$$

i.e.

$$0 \leq M_1 - 2m - mk_4 \leq \sqrt{(m-1)(mEM_1 - (M_1 - 2m)^2)}$$

wherefrom follows

$$EM_1 \geq \frac{(M_1 - 2m)^2}{m} + \frac{(M_1 - 2m - mk_4)^2}{m(m-1)}. \tag{25}$$

From the inequality

$$\begin{aligned} mEM_1 - (M_1 - 2m)^2 &= m\sum_{i=1}^{m} d(e_i)^2 - \left(\sum_{i=1}^{m} d(e_i)\right)^2 = \sum_{1\leq i<j\leq m} (d(e_i) - d(e_j))^2 \geq \\ &\geq \sum_{i=2}^{m-1}((d(e_1) - d(e_i))^2 + (d(e_i) - d(e_m))^2) + (d(e_1) - d(e_m))^2 \\ &\geq \frac{m}{2}(d(e_1) - d(e_m))^2, \end{aligned}$$

follows

$$EM_1 \geq \frac{(M_1 - 2m)^2}{m} + \frac{1}{2}(d(e_1) - d(e_m))^2. \tag{26}$$

The inequality (22) is obtained from the inequalities (24), (25) and (26). □

For $k_3 = d(e_1)$ and $k_4 = d(e_m)$ the following corollary holds.

Corollary 3.16. *Let G be a simple graph with n ($n \geq 2$) vertices and m edges. Then*

$$EM_1 \geq \frac{(M_1 - 2m)^2}{m} + \alpha(d(e_1), d(e_m)), \tag{27}$$

where

$$\alpha(d(e_1), d(e_m)) = \max\left\{\frac{(md(e_1) - M_1 + 2m)^2}{m(m-1)}, \frac{(M_1 - 2m - md(e_m))^2}{m(m-1)}, \frac{1}{2}(d(e_1) - d(e_m))^2\right\}.$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Remark 3.17. *The inequality (22), as well as the inequalities (24), (25) and (26), are stronger than (7).*

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