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REMARKS ON FIRST ZAGREB INDICES[1]

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Let G be an undirected connected graph with $n \geqslant 2$ vertices and m edges. In this paper we are concerned with inequalities that reveal connections between graph invariants called first Zagreb index and reformulated first Zagreb index. Some of the obtained results represent generalization of the known inequalities.

Key words: vertex degree, edge degree, first Zagreb index.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be undirected connected graph, where $V = \{1, 2, \ldots, n\}$ is set of vertices and $E = \{e_1, e_2, \ldots, e_m\}$ set of edges. Further, denote with $d_1 \geqslant d_2 \geqslant \ldots \geqslant d_n$, $d_i = d(i)$, $i = 1, 2, \ldots, n$, a sequence of vertex degrees of G. If $e = \{i, j\} \in E$, then $d(e) = d_i + d_j - 2$. The first Zagreb index M_1 and reformulated Zagreb index EM_1 are, respectively, defined by [8, 9]

$$M_1 = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad EM_1 = \sum_{i=1}^{m} d(e_i)^2.$$

If G is a graph and $L(G)$ is a corresponding line graph, then the following equality is valid $EM_1(G) = M_1(L(G))$. Invariants M_1 and EM_1 play an important role in algebraic graph theory, as well as in other sciences especially in molecular chemistry (see [2, 5, 6, 8, 9, 12]). Since these invariants can be calculated for a few classes of graphs in a closed form, it is of interest to find out inequalities that determine upper and lower bounds of these invariants in terms of some graph parameters or their mutual relationship. This is the topic of this paper.

We first give two inequalities that establish a connection between M_1 and EM_1 proved in [5].

Theorem 1.1. *Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be undirected connected graph with n vertices and m edges. Then*

$$EM_1 \geqslant \frac{(M_1 - 2m)^2}{m}, \tag{1}$$

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

Theorem 1.2. *Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be undirected connected graph with n vertices and m edges. Then*

$$EM_1 \leqslant \frac{(M_1 - 2m)^2 (d_1 + d_n - 2)^2}{4m(d_1 - 1)(d_n - 1)}, \tag{2}$$

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where $d_n \geqslant 2$, *with equality if and only if* G *is a regular graph or there are exactly* $\frac{m(d_n-1)}{d_1+d_n-2}$ *edges of degree* $2(d_1-1)$ *and* $\frac{m(d_1-1)}{d_1+d_n-2}$ *edges of degree* $2(d_n-1)$ *such that* (d_1+d_n-2) *divides* $m(d_n-1)$.

2. Main Result

The following theorem establishes a connection between invariants EM_1 and M_1 in terms of parameters m, d_1 and d_n.

Theorem 2.1. *Let* $G=(V,E)$, $V=\{1,2,\ldots,n\}$, $E=\{e_1,e_2,\ldots,e_m\}$, *be an undirected connected graph. Then*

$$\frac{(M_1-2m)^2}{m}+2(d_1-d_n)^2 \leqslant EM_1 \leqslant \frac{(M_1-2m)^2}{m}+4m(d_1-d_n)^2\alpha(m), \tag{3}$$

where

$$\alpha(m)=\frac{1}{m}\left\lfloor\frac{m}{2}\right\rfloor\left(1-\frac{1}{m}\left\lfloor\frac{m}{2}\right\rfloor\right)=\frac{1}{4}\left(1-\frac{(-1)^{m+1}+1}{2m^2}\right).$$

Equality holds if and only if $L(G)$ *is a regular graph.*

$\lhd$ The following inequality was proved in [1] for positive real numbers $p_1,p_2,\ldots,p_n$, $a_1,a_2,\ldots,a_n$ and $b_1,b_2,\ldots,b_n$ with the properties $0<r_1\leqslant a_i\leqslant R_1<+\infty$ and $0<r_2\leqslant b_i\leqslant R_2<+\infty$

$$\left|\sum_{i=1}^n p_i\sum_{i=1}^n p_ia_ib_i-\sum_{i=1}^n p_ia_i\sum_{i=1}^n p_ib_i\right| \leqslant (R_1-r_1)(R_2-r_2)\sum_{i\in S}p_i\left(\sum_{i=1}^n p_i-\sum_{i\in S}p_i\right), \tag{4}$$

where S is a subset of $I_n=\{1,2,\ldots,n\}$ for which the expression

$$\left|\sum_{i\in S}p_i-\frac{1}{2}\sum_{i=1}^n p_i\right| \tag{5}$$

reaches a minimal value.

For $n=m$ and $S=\{1,2,\ldots,k\}\subset I_m=\{1,2,\ldots m\}$ from (5) we obtain that $k=\lfloor\frac{m}{2}\rfloor$. Now, for $n=m$, $p_i=1$, $S=\{1,2,\ldots,\lfloor\frac{m}{2}\rfloor\}$, $a_i=b_i=d(e_i)$, $i=1,2,\ldots,m$, $R_1=R_2=2(d_1-1)$, $r_1=r_2=2(d_n-1)$ the inequality (4) becomes

$$m\sum_{i=1}^m d(e_i)^2-\left(\sum_{i=1}^m d(e_i)\right)^2 \leqslant 4(d_1-d_n)^2\left\lfloor\frac{m}{2}\right\rfloor\left(m-\left\lfloor\frac{m}{2}\right\rfloor\right). \tag{6}$$

Since $\sum_{i=1}^m d(e_i)=\sum_{i=1}^n d_i^2-2m=M_1-2m$, from (6) immediately follows right side of inequality (3).

Since the equality in (6) holds if and only if $d(e_1)=d(e_2)=\ldots=d(e_m)$, therefore equality on the right side of (3) holds if and only if $L(G)$ is a regular graph.

For the real numbers $a_1,a_2,\ldots,a_m$ with the property $r\leqslant a_i\leqslant R$, $i=1,2,\ldots,m$, the following inequality was proved in [10] (see also [11])

$$\sum_{i=1}^m\left(a_i-\frac{1}{m}\sum_{i=1}^m a_i\right)^2 \geqslant \frac{(R-r)^2}{2}.$$

For $a_i = d(e_i)$, $i = 1, 2, \dots, m$, $r = 2(d_n - 1)$ and $R = 2(d_1 - 1)$ the above inequality transforms into

$$\sum_{i=1}^{m}\left(d(e_i) - \frac{1}{m}\sum_{i=1}^{m} d(e_i)\right)^2 \geqslant 2(d_1 - d_n)^2, \tag{7}$$

i. e.

$$\sum_{i=1}^{m} d(e_i)^2 - \frac{1}{m}\left(\sum_{i=1}^{m} d(e_i)\right)^2 \geqslant 2(d_1 - d_n)^2,$$

where from the left side of inequality (3) is obtained.

Equality in (7) holds if and only if $d(e_1) = d(e_2) = \ldots = d(e_m)$, so the equality in the left part of (3) holds if and only if $L(G)$ is a regular graph. ▷

REMARK 2.1. Since $(d_1 - d_n)^2 \geqslant 0$, left inequality in (3) is stronger than inequality (1).

Corollary 2.1. *Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$ be an undirected connected graph. Then*

$$\frac{2\sqrt{2}}{\sqrt{m}}(M_1 - 2m)(d_1 - d_n) \leqslant EM_1 \leqslant \frac{(M_1 - 2m)^2}{m} + m(d_1 - d_n)^2. \tag{8}$$

Equality on the right side holds if and only if $L(G)$ is a regular graph. Equality on the left side holds if and only if $G = K_2$.

◁ Inequality on the left side in (8) is obtained from the left side of inequality (3) and inequality between arithmetic and geometric mean for real numbers. The right side of inequality (8) is obtained from the right part of inequality (3) and inequality $\alpha(m) \leqslant \frac{1}{4}$. ▷

Corollary 2.2. *Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$ be an undirected connected graph. Then*

$$4m(d_n - 1)^2 + 2(d_1 - d_n)^2 \leqslant EM_1 \leqslant 4m(d_1 - 1)^2 + 4m(d_1 - d_n)^2\alpha(m). \tag{9}$$

Equalities hold if and only if G is a regular graph.

◁ Inequalities (9) are obtained according to the inequality (3) and inequality

$$2m(d_n - 1) \leqslant M_1 - 2m \leqslant 2m(d_1 - 1). \quad ▷$$

Corollary 2.3. *Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be an undirected connected graph. Then*

$$4m\left(\frac{2m}{n} - 1\right)^2 + 2(d_1 - d_n)^2 \leqslant EM_1 \leqslant \frac{m}{(n-1)^2}\big(2m + (n-1)(n-4)\big)^2 + 4m(d_1 - d_n)\alpha(m).$$

Equality on the left side holds if and only if G is a regular graph. Equality on the right side holds if and only if G is a complete graph, i. e. $G = K_n$.

◁ The result immediately follows from inequality (3) and inequalities $M_1 \geqslant \frac{4m^2}{n}$, proved in [7], and $M_1 \leqslant m\big(\frac{2m}{n-1} + (n-2)\big)$, proved in [4]. ▷

Theorem 2.2. *Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be an undirected connected graph. Then*

$$EM_1 \leqslant (M_1 - 2m)(d_1 + d_n - 2) - 4m(d_1 - 1)(d_n - 1). \tag{10}$$

Equality holds if and only if G is a regular graph or a graph with the property that for some k, $1 \leqslant k \leqslant n$, sequence of vertex degrees is of the form $d_1 = d_2 = \ldots = d_k > d_{k+1} = d_{k+2} = \ldots = d_n$.

$\lhd$ For the real numbers $a_1, a_2, \ldots, a_m$ with the property $r \leqslant a_i \leqslant R$, $i = 1, 2, \ldots, m$, the following inequality was proved in [3] (see also [11])

$$\frac{1}{m}\sum_{i=1}^{m}\left(a_i - \frac{1}{m}\sum_{i=1}^{m} a_i\right)^2 \leqslant \left(R - \frac{1}{m}\sum_{i=1}^{m} a_i\right)\left(\frac{1}{m}\sum_{i=1}^{m} a_i - r\right).$$

For $a_i = d(e_i)$, $i = 1, 2, \ldots, m$, $r = 2(d_n - 1)$ and $R = 2(d_1 - 1)$ the above inequality becomes

$$\frac{1}{m}\sum_{i=1}^{m}\left(d(e_i) - \frac{1}{m}\sum_{i=1}^{m} d(e_i)\right)^2 \leqslant \left(2(d_1 - 1) - \frac{1}{m}\sum_{i=1}^{m} d(e_i)\right)\left(\frac{1}{m}\sum_{i=1}^{m} d(e_i) - 2(d_n - 1)\right),$$

i. e.

$$\frac{1}{m}\sum_{i=1}^{m} d(e_i)^2 \leqslant 2(d_1 + d_n - 2)\sum_{i=1}^{m} d(e_i) - 4(d_1 - 1)(d_n - 1),$$

where from the assertion of the theorem is obtained. $\rhd$

Remark 2.2. According to (10) the following inequality is valid

$$EM_1 + 4m(d_1 - 1)(d_n - 1) \leqslant 2(M_1 - 2m)(d_1 + d_n - 2). \tag{11}$$

Based on the inequality between arithmetic and geometric means for real numbers and applying it on the left part of inequality (11), the inequality

$$2\sqrt{4m(d_1 - 1)(d_n - 1)EM_1} \leqslant 2(M_1 - 2m)(d_1 + d_n - 2), \quad d_n > 1,$$

is obtained, i. e.

$$EM_1 \leqslant \frac{(M_1 - 2m)^2(d_1 + d_n - 2)^2}{4m(d_1 - 1)(d_n - 1)}.$$

This means that inequality (10) is stronger than inequality (2).

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ЗАМЕТКА О ПЕРВЫХ ЗАГРЕБСКИХ ИНДЕКСАХ

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Доказаны неравенства, связывающие первый и модифицированный первый загребские индексы графа. Для этих инвариантов графа доказаны неравенства, которые определяют их нижние и верхние границы. Эти неравенства улучшают некоторые известные результаты.

Ключевые слова: степень вершин, степень грани, первый загребский индекс.