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A Remark on the First Zagreb Index

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1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be a simple connected graph with $n \geq 3$ vertices and m edges. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $d_i = d(i)$, $i = 1, 2, \ldots, n$, a sequence of its vertex degrees. If vertices i and j are adjacent, we write $i \sim j$. Denote by $\mathbf{A}$ the adjacency matrix of G and by $\mathbf{D} = \mathrm{diag}\{d_1, d_2, \ldots, d_n\}$ the diagonal matrix of its vertex degrees. Then the Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$. Its eigenvalues, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, form the so called Laplacian spectrum of G. Some well known properties of these eigenvalues are [5]:

$$\sum_{i=1}^{n-1} \mu_i = \sum_{i=1}^{n} d_i = 2m \qquad \text{and} \qquad \sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1 + 2m,$$

where

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i \sim j} (d_i + d_j),$$

is the first Zagreb index introduced in [10]. A topological index, or graph invariant, for a graph is a numerical quantity which is invariant under automorphisms of the graph. For details on chemical and other applications of the first Zagreb index see for example [1–3, 7–9, 11, 16, 17, 20, 24, 29] and the references cited therein.

In this paper we establish new upper and lower bounds for the invariant M_1.

2. Preliminaries

In this section we recall some results from the spectral graph theory needed for the subsequent considerations.

In [6] (see also [12, 23, 25]) the following results were proved:

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Lemma 1. *[6] Let G be a connected graph with n vertices and m edges. Then*

$$M_1 \geq \frac{4m^2}{n}. \tag{1}$$

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

Lemma 2. [4] *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$M_1 \leq m\left(\frac{2m}{n-1} + n - 2\right). \tag{2}$$

Equality holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Lemma 3. [18] *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$\sqrt{\frac{(n-1)(M_1+2m)-4m^2}{(n-1)^2\alpha(n-1)}} \leq \mu_1 - \mu_{n-1} \leq \leq \sqrt{\frac{2((n-1)(M_1+2m)-4m^2)}{n-1}}, \tag{3}$$

where

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

Equalities hold if and only if $G \cong K_n$.

Let us note that left part of the inequality (3) was proved in [13], and right part in [19], but in a different way.

3. Main result

We will first prove one auxiliary result for the lower and upper bounds of the Laplacian eigenvalues μ_i, $i = 1, 2, \ldots, n-1$.

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

$$\frac{2m}{n-1} + \frac{1}{n-1}\sqrt{\frac{(n-1)(M_1+2m)-4m^2}{n-2}} \leq \mu_1 \leq \frac{2m}{n-1} + \frac{1}{n-1}\sqrt{(n-2)((n-1)(M_1+2m)-4m^2)}, \tag{4}$$

$$\frac{2m}{n-1} - \frac{1}{n-1}\sqrt{\frac{(i-1)((n-1)(M_1+2m)-4m^2)}{n-i}} \leq \mu_i \leq \frac{2m}{n-1} + \frac{1}{n-1}\sqrt{\frac{(n-i-1)((n-1)(M_1+2m)-4m^2)}{i}}, \quad 2 \leq i \leq n-2, \tag{5}$$

$$\frac{2m}{n-1} - \frac{1}{n-1}\sqrt{(n-2)((n-1)(M_1+2m)-4m^2)} \leq \mu_{n-1} \leq \frac{2m}{n-1} - \frac{1}{n-1}\sqrt{\frac{(n-1)(M_1+2m)-4m^2}{n-2}}. \tag{6}$$

Equalities hold if and only if $G \cong K_n$.

Proof. In [15] a class of real polynomials of type $\mathcal{P}_n(a_1, a_2)$ 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. It was proved that for the roots of polynomials of that class the following inequalities are valid

$$\begin{aligned} &\bar{x} + \frac{1}{n}\sqrt{\frac{\Delta}{n-1}} \le x_1 \le \bar{x} + \frac{1}{n}\sqrt{(n-1)\Delta}, \\ &\bar{x} - \frac{1}{n}\sqrt{\frac{i-1}{n-i+1}\Delta} \le x_i \le \bar{x} + \frac{1}{n}\sqrt{\frac{n-i}{i}\Delta}, \quad 2 \le i \le n-1, \\ &\bar{x} - \frac{1}{n}\sqrt{(n-1)\Delta} \le x_n \le \bar{x} - \frac{1}{n}\sqrt{\frac{\Delta}{n-1}}, \end{aligned} \tag{7}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \text{and} \qquad \Delta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2. \tag{8}$$

Now consider the Laplacian characteristic polynomial of the graph G

$$\begin{aligned} \bar{\varphi}_n(x) &= x\varphi_{n-1}(x) = x\prod_{i=1}^{n-1}(x - \mu_i) = \\ &= x\left(x^{n-1} + a_1x^{n-2} + a_2x^{n-2} + b_3x^{n-3} + \cdots + b_{n-1}\right). \end{aligned}$$

Since

$$\begin{aligned} a_1 &= -\sum_{i=1}^{n-1}\mu_i = -2m \quad \text{and} \\ a_2 &= \frac{1}{2}\left(\left(\sum_{i=1}^{n-1}\mu_i\right)^2 - \sum_{i=1}^{n-1}\mu_i^2\right) = 2m^2 - m - \frac{1}{2}M_1, \end{aligned}$$

the polynomial $\varphi_{n-1}(x)$ belongs to a class of real polynomials $\mathcal{P}_{n-1}(-2m, 2m^2 - m - \frac{1}{2}M_1)$. According to (8), for its roots $\mu_1, \mu_2, \ldots, \mu_{n-1}$, holds

$$\bar{x} = \frac{1}{n-1}\sum_{i=1}^{n-1}\mu_i = \frac{2m}{n-1}$$

and

$$\Delta = (n-1)\sum_{i=1}^{n-1}\mu_i^2 - \left(\sum_{i=1}^{n-1}\mu_i\right)^2 = (n-1)(M_1 + 2m) - 4m^2.$$

From the above identities and (7) we obtain the required result. □

Remark 1. *Right hand side of the inequality (4) was proved in [22] (see also [21]). Left hand side of (6) was proved in [22] (see also [23]).*

Remark 2. *If in (4), (5) and (6) M_1 is substituted by its upper and lower bounds, then lower and upper bounds for μ_i, $i = 1, 2, \ldots, n-1$ in terms of various graph parameters (e.g. n, m, d_i, etc.) can be obtained. Thus, for example, if* *we replace M_1 with its boundaries given by (1) and (2), in (4), (5) and (6), the following boundaries for μ_i are obtained*

$$\begin{aligned}&\frac{2m}{n-1}+\frac{1}{n-1}\sqrt{\frac{2m(n(n-1)-2m)}{n(n-2)}}\le \mu_1 \le\\ &\frac{2m}{n-1}+\frac{1}{n-1}\sqrt{m(n-2)(n(n-1)-2m)},\end{aligned} \tag{9}$$

$$\begin{aligned}&\frac{2m}{n-1}-\frac{1}{n-1}\sqrt{\frac{(i-1)m(n(n-1)-2m)}{n-i}}\le \mu_i \le\\ &\frac{2m}{n-1}+\frac{1}{n-1}\sqrt{\frac{(n-i-1)m(n(n-1)-2m)}{i}},\ \ 2\le i\le n-2,\end{aligned} \tag{10}$$

$$\begin{aligned}&\frac{2m}{n-1}-\frac{1}{n-1}\sqrt{m(n-2)(n(n-1)-2m)}\le \mu_{n-1} \le\\ &\frac{2m}{n-1}-\frac{1}{n-1}\sqrt{\frac{2m(n(n-1)-2m)}{n(n-2)}}.\end{aligned} \tag{11}$$

Equalities hold if and only if $G \cong K_n$.

Right hand side of inequality (9) was proved in [14] (see also [27]), and the left part in [26]. Right hand side of (10) was proved in [28], and left part in [26]. Right hand side of (11) was proved in [26], and left hand side in [27] (see also [23]).

Denote by k_1, k_2, k_3, k_4 real numbers with the properties

$$\begin{aligned}&\mu_1 \ge k_1 \ge \frac{2m}{n-1},\quad \frac{2m}{n-1}\ge k_2 \ge \mu_{n-1},\\ &k_3 \ge \mu_1,\quad 0\le k_4\le \mu_{n-1}\,,\end{aligned} \tag{12}$$

and let

$$\beta(k_1,k_2)=\max\left\{\frac{((n-1)k_1-2m)^2}{(n-1)(n-2)},\frac{(2m-(n-1)k_2)^2}{(n-1)(n-2)},\frac{1}{2}(\mu_1-\mu_{n-1})^2\right\},$$

and

$$\begin{aligned}\gamma(k_3,k_4)\ \ =\ \ &\min\left\{\frac{(n-2)((n-1)k_3-2m)^2}{n-1},\frac{(n-2)(2m-(n-1)k_4)^2}{n-1},\right.\\ &\left.(n-1)\alpha(n-1)(\mu_1-\mu_{n-1})^2\right\}.\end{aligned}$$

Theorem 1. *Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then*

$$\frac{2m(2m-n+1)}{n-1}+\beta(k_1,k_2)\le M_1\le \frac{2m(2m-n+1)}{n-1}+\gamma(k_3,k_4). \tag{13}$$

Equalities hold if and only if $G \cong K_n$.

Proof. For any real k_1 with the property $\mu_1 \ge k_1 \ge \frac{2m}{n-1}$, based on the right hand side of inequality (4), the following inequality is valid

$$k_1\le\mu_1\le\frac{2m}{n-1}+\frac{1}{n-1}\sqrt{(n-2)((n-1)(M_1+2m)-4m^2)},$$

that is

$$((n-1)k_1-2m)^2 \le (n-2)(n-1)M_1-2m(n-2)(2m-n+1),$$

wherefrom follows

$$M_1 \ge \frac{2m(2m-n+1)}{n-1}+\frac{((n-1)k_1-2m)^2}{(n-1)(n-2)}. \tag{14}$$

For any real k_2 with the property $\frac{2m}{n-1} \ge k_2 \ge \mu_{n-1}$, from the left hand side of (6) we have that

$$\frac{2m}{n-1}-\frac{1}{n-1}\sqrt{(n-2)((n-1)(M_1+2m)-4m^2)} \le \mu_{n-1} \le k_2,$$

i.e.

$$(2m-(n-1)k_2)^2 \le (n-2)(n-1)M_1-2m(n-2)(2m-n+1),$$

wherefrom follows

$$M_1 \ge \frac{2m(2m-n+1)}{n-1}+\frac{(2m-(n-1)k_2)^2}{(n-1)(n-2)}. \tag{15}$$

The inequalities (3) can be rewritten in the following form

$$\begin{aligned}\frac{2m(2m-n+1)}{n-1}+\frac{1}{2}(\mu_1-\mu_{n-1})^2 \le M_1 \le \\ \le \frac{2m(2m-n+1)}{n-1}+(n-1)\alpha(n-1)(\mu_1-\mu_{n-1})^2.\end{aligned} \tag{16}$$

The left part of inequality (13) is obtained according to (14), (15) and the left side of (16).
The right part of (13) can be proved similarly. □

For $k_1=k_3=\mu_1$ and $k_2=k_4=\mu_{n-1}$ the following corollary of Theorem 1 is valid.

Corollary 1. *Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then*

$$\frac{2m(2m-n+1)}{n-1}+\beta(\mu_1,\mu_{n-1}) \le M_1 \le \frac{2m(2m-n+1)}{n-1}+\gamma(\mu_1,\mu_{n-1}),$$

where

$$\beta(\mu_1,\mu_{n-1}) = \max\left\{\frac{((n-1)\mu_1-2m)^2}{(n-1)(n-2)}, \frac{(2m-(n-1)\mu_{n-1})^2}{(n-1)(n-2)}, \frac{1}{2}(\mu_2-\mu_{n-1})^2\right\}$$

and

$$\begin{aligned}\gamma(\mu_1,\mu_{n-1}) \quad = \quad & \min\left\{\frac{(n-2)((n-1)\mu_1-2m)^2}{n-1}, \frac{(n-2)(2m-(n-1)\mu_{n-1})^2}{n-1},\right. \\ & \left.(n-1)\alpha(n-1)(\mu_1-\mu_{n-1})^2\right\}.\end{aligned}$$

Equalities hold if and only if $G \cong K_n$.

For $k_1=k_2=\frac{2m}{n-1}$ the following corollary of Theorem 1 is valid.

Corollary 2. *Let G be a simple connected graph with $n \ge 3$ vertices and m edges. Then*

$$M_1 \ge \frac{2m(2m-n+1)}{n-1}+\frac{1}{2}(\mu_1-\mu_{n-1})^2. \tag{17}$$

Equality holds if and only if $G \cong K_n$.

Let us note that inequality (17) was proved in [19].

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