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SOME INEQUALITIES FOR THE HARMONIC TOPOLOGICAL INDEX

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Abstract. Let G be a simple connected graph with n vertices and m edges, with a sequence of vertex degrees $d_1 \geq d_2 \geq \cdots \geq d_n > 0$. A vertex-degree topological index, referred to as harmonic index, is defined as $H = \sum_{i \sim j} \frac{2}{d_i + d_j}$, where $i \sim j$ denotes the adjacency of vertices i and j. Lower and upper bounds of the index H are obtained.

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1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple connected graph with n vertices and m edges. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m) > 0$, sequences of vertex and edge degrees, respectively. If i-th and j-th vertices (e_i and e_j edges) are adjacent, we write $i \sim j$ ($e_i \sim e_j$). In addition, we use the following notation: $\Delta = d_1$, $\delta = d_n$, $\Delta_e = d(e_1) + 2$, $\delta_e = d(e_m) + 2$, $\Delta_{e_2} = d(e_2) + 2$, $\delta_{e_2} = d(e_{m-1}) + 2$. As usual, $L(G)$ denotes a line graph.

Gutman and Trinajstić [8] introduced two vertex-degree topological indices, named as the first, and the second Zagreb index, M_1 and M_2, defined as

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

The first Zagreb index can be also expressed as (see [4])

$$M_1 = \sum_{i \sim j} (d_i + d_j). \tag{1}$$

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Details on the first Zagreb index and its applications can be found in [1, 2, 3, 7, 9, 10, 11].

Zhou and Trinajstić [26] defined general sum-connectivity index H_α, as

$$H_\alpha = H_\alpha(G) = \sum_{i\sim j}(d_i + d_j)^\alpha, \tag{2}$$

where α is an arbitrary real number.

Here we are concerned with two special cases of the invariant H_α. These are sum-connectivity index X, defined in [25] as

$$X = X(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_i + d_j}}, \tag{3}$$

and harmonic index H [6]

$$H = H(G) = \sum_{i\sim j} \frac{2}{d_i + d_j}. \tag{4}$$

In this paper we state some new inequalities that set up upper and lower bounds for the invariant H. For more details of harmonic index see in [12, 13, 14, 19, 20, 22, 23, 24].

2. Preliminaries

In this section we recall some results for the invariant H and real number sequences that will be used in the subsequent considerations.

In [19] Rodriguez and Sigarreta determined the upper bound for the index H in terms of invariant M_1 and graph parameters m, Δ and δ

$$H \le \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2, \tag{5}$$

with equality holding if G is a regular graph.

Ilić [13] and Xu [22] independently obtained the following inequality

$$H \ge \frac{2m^2}{M_1}, \tag{6}$$

with equality if and only if $d_i + d_j$ is constant for each pair of adjacent vertices i and j.

Let $p = (p_i)$, and $a = (a_i)$, $i = 1, 2, \ldots, m$, be two non-negative real number sequences with the properties

$$p_1 + p_2 + \cdots + p_m = 1 \quad \text{and} \quad 0 < r \le a_i \le R < +\infty.$$

In [18] (see also [16]) Rennie proved that

$$\sum_{i=1}^{m} p_i a_i + rR\sum_{i=1}^{m} \frac{p_i}{a_i} \le r + R, \tag{7}$$

with equality if and only if for arbitrary k, $1 \le k \le m-1$, holds $R = a_1 = \cdots = a_k \ge a_{k+1} = \cdots = a_m = r$, or $R = a_1 = \cdots = a_m = r$.

In [21] (see also [17]) the following was proved:

Let $p = (p_i)$, $i = 1, 2, \ldots, m$, be positive real number sequence, and $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, m$, sequences of non-negative real numbers of similar monotonicity. Denote with

$$T_m(a, b; p) = \sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i.$$

Then

$$T_m(a, b; p) \ge T_{m-1}(a, b; p). \tag{8}$$

The inequality $T_m(a, b; p) \ge 0$ is well-known Chebyshev inequality (see for example [16]).

3. Main results

In the following theorem we prove the inequality that establishes upper bound for H in terms of m, Δ_e, δ_e and M_1.

Theorem 3.1. *Let G be a simple connected graph with n vertices and $m \ge 2$ edges. Then*

$$H \le \frac{2(m(\Delta_e + \delta_e) - M_1)}{\Delta_e \delta_e}. \tag{9}$$

Equality holds if and only if $L(G)$ is a regular graph, or for arbitrary k, $1 \le k \le m-1$, holds $\Delta_e = d(e_1)+2 = \cdots = d(e_k)+2 \ge d(e_{k+1})+2 = \cdots = d(e_m)+2 = \delta_e$.

Proof. For $p_i = \frac{1}{m}$, $a_i = d(e_i) + 2$, $i = 1, 2, \ldots, m$, $R = d(e_1) + 2 = \Delta_e$, and $r = d(e_m) + 2 = \delta_e$, inequality (7) becomes

$$\frac{1}{m} \sum_{i=1}^{m} (d(e_i) + 2) + \frac{\Delta_e \delta_e}{m} \sum_{i=1}^{m} \frac{1}{d(e_i) + 2} \le \Delta_e + \delta_e. \tag{10}$$

According to (1) and (4) topological indices M_1 and H can be expressed as

$$M_1 = \sum_{i=1}^{m} (d(e_i) + 2) \quad \text{and} \quad H = \sum_{i=1}^{m} \frac{2}{d(e_i) + 2}. \tag{11}$$

From (10) and (11) we have

$$2M_1 + \Delta_e \delta_e H \le 2m(\Delta_e + \delta_e), \tag{12}$$

wherefrom (9) is obtained.

Equality in (7) holds if and only if $R = a_1 = \cdots = a_m = r$, or for arbitrary k, $1 \le k \le m-1$, holds $R = a_1 = \cdots = a_k \ge a_{k+1} = \cdots = a_m = r$. Therefore equality in (9) holds if and only if $L(G)$ is a regular graph, or for arbitrary k, $1 \le k \le m-1$, holds $\Delta_e = d(e_1) + 2 = \cdots = d(e_k) + 2 \ge d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_e$. □

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

$$H \leq \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta_e}{\delta_e}}+\sqrt{\frac{\delta_e}{\Delta_e}}\right)^2 . \tag{13}$$

Equality holds if $L(G)$ is regular.

Proof. According to the arithmetic-geometric mean inequality for non-negative real numbers (see for example [16]), from (12) we get

$$2\sqrt{2\Delta_e\delta_e H M_1} \leq 2M_1 + \Delta_e\delta_e H \leq 2m(\Delta_e+\delta_e),$$

wherefrom the inequality (13) is obtained. □

Corollary 3.3. *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$H \leq \frac{nm^2}{8m^2+n(\Delta-\delta)^2}\left(\sqrt{\frac{\Delta_e}{\delta_e}}+\sqrt{\frac{\delta_e}{\Delta_e}}\right)^2 .$$

Equality holds if G is regular.

Proof. The inequality is obtained from (13) and inequality

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

which was proved in [15]. □

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

$$H \leq \frac{2m(n(\Delta_e+\delta_e)-4m)}{n\Delta_e\delta_e}.$$

Equality holds if G is regular.

Proof. This inequality can be obtained according to (9) and inequality

$$M_1 \geq \frac{4m^2}{n}, \tag{14}$$

proved in [5]. □

Remark 3.1. The function $f(x) = x + \frac{1}{x}$ is increasing for $x \geq 1$. Since $2\delta \leq \delta_e \leq \Delta_e \leq 2\Delta$, we have $1 \leq \frac{\Delta_e}{\delta_e} \leq \frac{\Delta}{\delta}$. According to (13) we get

$$H \leq \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta_e}{\delta_e}}+\sqrt{\frac{\delta_e}{\Delta_e}}\right)^2 \leq \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)^2 .$$

Therefore inequality (13) is stronger than (5).

Remark 3.2. From the definition of invariant H it follows

$$\frac{2m}{\Delta_e} \leq H \leq \frac{2m}{\delta_e},$$

with equalities if and only if $L(G)$ is regular graph. Since $\frac{2m}{\delta_e} \leq \frac{2m}{2\delta} \leq m$ and $\frac{2m}{\Delta_e} \geq \frac{2m}{2\Delta} \geq \frac{m}{n-1}$, these inequalities are stronger than

$$\frac{m}{n-1} \leq H \leq m,$$

proved in [20].

By a similar procedure as in case of Theorem 3.1, the following can be proved.

Theorem 3.5. *Let G be a simple connected graph with n vertices and m edges. If $m \geq 3$, then*

$$H \leq \frac{2}{\Delta_e} + \frac{2((m-1)(\Delta_{e_2} + \delta_e) - M_1 + \Delta_e)}{\Delta_{e_2}\delta_e}.$$

Equality holds if and only if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_m) + 2 = \delta_e$, or for arbitrary k, $2 \leq k \leq m-1$, $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_e$.

If $m \geq 3$, then

$$H \leq \frac{2}{\delta_e} + \frac{2((m-1)(\Delta_e + \delta_{e_2}) - M_1 + \delta_e)}{\Delta_e\delta_{e_2}}.$$

Equality holds if and only if $\Delta_e = d(e_1) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$, or for arbitrary k, $1 \leq k \leq m-2$, $\Delta_e = d(e_1) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$.

If $m \geq 4$, then

$$H \leq \frac{2(\Delta_e + \delta_e)}{\Delta_e\delta_e} + \frac{2((m-2)(\Delta_{e_2} + \delta_{e_2}) - M_1 + \Delta_e + \delta_e)}{\Delta_{e_2}\delta_{e_2}}.$$

Equality holds if and only if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$, or for arbitrary k, $2 \leq k \leq m-2$, $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$.

In the next theorem we prove inequality which establishes a connection between topological indices H and X.

Theorem 3.6. *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$H \leq \frac{2((\sqrt{\Delta_e} + \sqrt{\delta_e})X - m)}{\sqrt{\Delta_e\delta_e}}. \tag{15}$$

Equality holds if and only if $L(G)$ is regular, or for arbitrary k, $1 \leq k \leq m-1$, holds $\Delta_e = d(e_1) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_e$.

Proof. For

$$p_i = \frac{\frac{1}{\sqrt{d(e_i)+2}}}{\sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}}}, \quad a_i = \sqrt{d(e_i)+2},$$

$i = 1, 2, \dots, m$, $r = \sqrt{\delta_e} = \sqrt{d(e_m)+2}$, and $R = \sqrt{\Delta_e} = \sqrt{d(e_1)+2}$, the inequality (7) becomes

$$\frac{m}{\sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}}} + \sqrt{\Delta_e \delta_e} \frac{\sum_{i=1}^{m} \frac{1}{d(e_i)+2}}{\sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}}} \leq \sqrt{\Delta_e} + \sqrt{\delta_e}. \tag{16}$$

According to (3), topological index X can be expressed as

$$X = \sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}}. \tag{17}$$

Now, from (11) and (17), the inequality (16) becomes

$$\frac{m}{X} + \sqrt{\Delta_e \delta_e} \frac{H}{2X} \leq \sqrt{\Delta_e} + \sqrt{\delta_e},$$

wherefrom (15) is obtained. This completes the proof. □

Corollary 3.7. *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$H \leq \frac{X^2 \left(\sqrt{\Delta_e} + \sqrt{\delta_e}\right)^2}{2m\sqrt{\Delta_e \delta_e}}. \tag{18}$$

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

In the following theorem we prove the inequality which is opposite to inequality (18).

Theorem 3.8. *Let G be a simple graph with n vertices and $m \geq 2$ edges. Then*

$$H \geq \frac{2X^2}{m} + \frac{2}{m} \left(\frac{1}{\sqrt{\Delta_{e_2}}} - \frac{1}{\sqrt{\Delta_e}} \right)^2. \tag{19}$$

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

Proof. From inequality (8) we have that

$$T_m(a, b; p) \geq T_2(a, b; p),$$

i.e.

$$\sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i \geq p_1 p_2 (a_1 - a_2)(b_1 - b_2).$$

For $p_i = 1$, $a_i = b_i = \frac{1}{\sqrt{d(e_i)+2}}$, $i = 1, 2, \ldots, m$, this inequality transforms into

$$m \sum_{i=1}^{m} \frac{1}{d(e_i)+2} - \left(\sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}} \right)^2 \geq \left(\frac{1}{\sqrt{d(e_2)+2}} - \frac{1}{\sqrt{d(e_1)+2}} \right)^2,$$

i.e.

$$\frac{1}{2} mH - X^2 \geq \left(\frac{1}{\sqrt{\Delta_{e_2}}} - \frac{1}{\sqrt{\Delta_e}} \right)^2,$$

wherefrom we obtain the statement of the theorem. □

Since

$$\left(\frac{1}{\sqrt{\Delta_{e_2}}} - \frac{1}{\sqrt{\Delta_e}} \right)^2 \geq 0,$$

we get the following corollary of Theorem 3.8.

Corollary 3.9. *Let G be a simple connected graph with n vertices and $m \geq 1$ edges. Then*

$$H \geq \frac{2X^2}{m}. \tag{20}$$

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

Remark 3.3. From (8) we get the Chebyshev inequality $T_m(a, b; p) \geq 0$, i.e.

$$\sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i \geq \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i. \tag{21}$$

If sequences $a = (a_i)$ and $b = (b_i)$ are of opposite monotonicity, then the sense of (21) reverses.

For $p_i = a_i = \sqrt{d(e_i)+2}$ and $b_i = \frac{1}{\sqrt{d(e_i)+2}}$, $i = 1, 2, \ldots, m$, the inequality (21) becomes

$$\left(\sum_{i=1}^{m} \sqrt{d(e_i)+2} \right)^2 \leq mM_1. \tag{22}$$

For $p_i = \sqrt{d(e_i)+2}$ and $a_i = b_i = \frac{1}{\sqrt{d(e_i)+2}}$, $i = 1, 2, \ldots, m$, the inequality (21) transforms into

$$\left(\sum_{i=1}^{m} \sqrt{d(e_i)+2} \right) X \geq m^2. \tag{23}$$

Now, according to (22) and (23), we have that

$$\frac{2X^2}{m} \geq \frac{2m^2}{M_1}.$$

Therefore the inequality (20) is stronger than (6).

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