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Some new upper bounds for the hyper-Zagreb index

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Abstract

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be a simple connected graph with n vertices, m edges, and degree sequence $(d_1, d_2, \cdots, d_n)$ where $d_1 \geq d_2 \geq \cdots \geq d_n > 0$. With $i \sim j$, we denote the adjacency of the vertices i and j in G. The hyper-Zagreb index of the graph G is defined as $HM = HM(G) = \sum_{i\sim j}(d_i + d_j)^2$. Some new upper bounds on the graph invariant HM are obtained here.

Keywords: hyper-Zagreb index; harmonic index; multiplicative sum Zagreb index; edge degree.

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1. Introduction

Let $G = (V, E)$ be a simple connected graph, where $V = \{1, 2, \ldots, n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$. The number of the first neighbors of a vertex $i \in V$ is called degree of the vertex i and is denoted by $d_i = d(i)$. The degree of an edge $e \in E$, connecting the vertices i and j, is defined as $d(e) = d_i + d_j - 2$. Denote by $(d_1, d_2, \cdots, d_n)$ and $(d(e_1), d(e_2), \cdots, d(e_m))$ the sequences of vertex and edge degrees, respectively, where $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$. If vertices i and j are adjacent we denote it as $i \sim j$. In addition, we use the following notation: $\Delta_e = d(e_1) + 2$ and $\delta_e = d(e_m) + 2$. As usual, $L(G)$ denotes a line graph of G.

A topological index, or graph invariant, for a graph, is a numerical quantity which remains invariant under graph isomorphism. Very often in chemistry, the aim is the construction of chemical compounds with certain properties, which not only depend on the chemical formula but also strongly on the molecular structure. That's where various topological indices come into consideration.

The first Zagreb index and the second Zagreb index, denoted by M_1 and M_2, respectively, are among the oldest vertex–degree–based topological indices. For a graph G, these indices are defined [15, 16] as

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

Details on the mathematical theory of the Zagreb indices can be found in [6, 7, 17, 18, 23].

As shown in [8] and [20], the first Zagreb index can be expressed as

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

and

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

A modification of the first Zagreb index, F, defined as the sum of third powers of vertex degrees, that is

$$F = F(G) = \sum_{i=1}^{n} d_i^3 ,$$

was first time encountered in 1972, in the paper [15], but was eventually disregarded. Recently, it was re-considered in [14] and named the forgotten index.

The hyper-Zagreb index, HM, defined as

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

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was put forwarded [26] in 2013. Since

$$F = \sum_{i \sim j} (d_i^2 + d_j^2),$$

it follows

$$HM = F + 2M_2.$$

One can easily verify that

$$HM = \sum_{i=1}^{m} (d(e_i) + 2)^2.$$

Another degree–based topological index is the ”harmonic index”, H, which was introduced in [13]. For a graph G, this index is defined as

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

The harmonic index, H, gained a considerable attention from mathematician after the publication of the paper [30]. Extremal results and bounds concerning the hyper-Zagreb index and harmonic index have recently been summarized in the survey [2].

In [27], multiplicative variants of the additive graph invariants were proposed. Using this idea, the authors of [9] proposed a multiplicative variant of (1) and called it as the multiplicative sum Zagreb index, and denoted it by Π_1^*. For a graph G, this invariant is defined as

$$\Pi_1^* = \Pi_1^*(G) = \prod_{i \sim j} (d_i + d_j).$$

Again, it is easily to verify that the following identities hold

$$H = \sum_{i=1}^{m} \frac{2}{d(e_i) + 2} \quad \text{and} \quad \Pi_1^* = \prod_{i=1}^{m} (d(e_i) + 2).$$

More on these and some other degree–based topological indices can be found, for example, in [1, 4, 5, 18, 27–29].

In [10–12, 24], various upper bounds for the hyper-Zagreb index, HM, were derived. In this paper, we establish some new upper bounds for HM, which depend on the parameters m, Δ_e, δ_e and some other graph invariants.

2. Preliminary results

In this section, we recall some discrete analytical inequalities for real number sequences that will be used in the subsequently.

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, m$, be positive real number sequences with the property $0 < r \le a_i \le R < +\infty$. Further, let S be a subset of $I_m = \{1, 2, \ldots, m\}$, $S \subset I_m$, which minimizes the expression

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

In [21] the following inequality was proven

$$\sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} \frac{p_i}{a_i} \le \left(1 + \gamma(S) \frac{(R-r)^2}{rR} \right) \left(\sum_{i=1}^{m} p_i \right)^2, \tag{3}$$

where

$$\gamma(S) = \frac{\sum_{i \in S} p_i}{\sum_{i=1}^{m} p_i} \left(1 - \frac{\sum_{i \in S} p_i}{\sum_{i=1}^{m} p_i} \right). \tag{4}$$

Let $p = (p_i)$ and $a = (a_i)$, $b = (b_i)$, $i = 1, 2, \ldots, m$, be positive real number sequences with the properties $0 < r_1 \le a_i \le R_1 < +\infty$ and $0 < r_2 \le b_i \le R_2 < +\infty$, and S be a subset of $I_m = \{1, 2, \ldots, m\}$ which minimizes the expression (2). In [3] it was proven

$$\left| \sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i \right| \le \gamma(S)(R_1 - r_1)(R_2 - r_2) \left(\sum_{i=1}^{m} p_i \right)^2, \tag{5}$$

where $\gamma(S)$ is given by (4).

Let $a=(a_i)$, $i=1,2,\dots,m$, be a positive real number sequence. In [19] the following inequalities were proven

$$\left(\sum_{i=1}^{m}\sqrt{a_i}\right)^2 \le (m-1)\sum_{i=1}^{m}a_i + m\left(\prod_{i=1}^{m}a_i\right)^{\frac{1}{m}} \tag{6}$$

and

$$\left(\sum_{i=1}^{m}\sqrt{a_i}\right)^2 \ge \sum_{i=1}^{m}a_i + m(m-1)\left(\prod_{i=1}^{m}a_i\right)^{\frac{1}{m}}. \tag{7}$$

Let $p=(p_i)$ and $a=(a_i)$, $i=1,2,\dots,m$, be two positive real number sequences with the properties $p_1+p_2+\cdots+p_m=1$ and $0<r\le a_i\le R<+\infty$. In [25] (see also [22]) it was proven

$$\sum_{i=1}^{m}p_ia_i + rR\sum_{i=1}^{m}\frac{p_i}{a_i} \le r+R. \tag{8}$$

3. Main results

In the following theorem we determine an upper bound for $HM(G)$ in terms of parameters m, Δ_e, δ_e and invariants $M_1(G)$, $H(G)$ and $\Pi_1^*(G)$.

Theorem 3.1. *Let G be a simple connected graph with $m\ge 1$ edges. Then*

$$HM(G) \le \frac{2(m-1)M_1(G)+2m(\Pi_1^*(G))^{\frac{1}{m}}}{H(G)} + \frac{\beta(S)\left(\Delta_e^{3/2}-\delta_e^{3/2}\right)^2 H(G)}{2}, \tag{9}$$

where

$$\beta(S) = \frac{\sum\limits_{i\in S}\frac{2}{d(e_i)+2}}{H(G)}\left(1-\frac{\sum\limits_{i\in S}\frac{2}{d(e_i)+2}}{H(G)}\right) \tag{10}$$

and S is a subset of $I_m=\{1,2,\dots,m\}$ which minimizes the expression

$$\left|\sum_{i\in S}\frac{2}{d(e_i)+2}-\frac{1}{2}H(G)\right|. \tag{11}$$

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

Proof. For $p_i=\frac{1}{d(e_i)+2}$, $i=1,2,\dots,m$, from (2) we obtain that S is a subset of $I_m=\{1,2,\dots,m\}$ which minimizes the expression (11), and according to (4) we have that $\gamma(S)=\beta(S)$, where $\beta(S)$ is given by (10). Further, for $p_i=\frac{1}{d(e_i)+2}$, $a_i=b_i=(d(e_i)+2)^{3/2}$, $R_1=R_2=\Delta_e^{3/2}$, $r_1=r_2=\delta_e^{3/2}$, $i=1,2,\dots,m$, the inequality (5) becomes

$$\sum_{i=1}^{m}\frac{1}{d(e_i)+2}\sum_{i=1}^{m}(d(e_i)+2)^2-\left(\sum_{i=1}^{m}\sqrt{d(e_i)+2}\right)^2$$
$$\le \beta(S)\left(\Delta_e^{3/2}-\delta_e^{3/2}\right)^2\left(\sum_{i=1}^{m}\frac{1}{d(e_i)+2}\right)^2,$$

that is

$$\frac{1}{2}H(G)HM(G) \le \left(\sum_{i=1}^{m}\sqrt{d(e_i)+2}\right)^2 + \frac{1}{4}\beta(S)\left(\Delta_e^{3/2}-\delta_e^{3/2}\right)^2 H(G)^2. \tag{12}$$

On the other hand, for $a_i=d(e_i)+2$, $i=1,2,\dots,m$, the inequality (6) transforms into

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

that is

$$\left(\sum_{i=1}^{m}\sqrt{d(e_i)+2}\right)^2 \le (m-1)M_1(G)+m\left(\Pi_1^*(G)\right)^{\frac{1}{m}}. \tag{13}$$

Now, by (12) and (13) it follows

$$\frac{1}{2}H(G)HM(G) \leq (m-1)M_1(G) + m(\Pi_1^*(G))^{\frac{1}{m}} + \frac{1}{4}\beta(S)\left(\Delta_e^{3/2} - \delta_e^{3/2}\right)^2 H(G)^2,$$

wherefrom (9) is obtained.

Equality in (6) holds if and only if $a_1 = a_2 = \cdots = a_m$, therefore equality in (13) holds if and only if $\Delta_e = d(e_1)+2 = d(e_2)+2 = \cdots = d(e_m)+2 = \delta_e$. This means that equality in (9) holds if and only if $\Delta_e = d(e_1)+2 = d(e_2)+2 = \cdots = d(e_m)+2 = \delta_e$, that is if and only if $L(G)$ is a regular graph. □

According to the arithmetic-geometric mean inequality for real numbers (see e.g. [22]), we have that for any set S, $S \subset I_m$, holds $\beta(S) \leq \frac{1}{4}$. Therefore, we have the following corollary of Theorem 3.1.

Corollary 3.1. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$HM(G) \leq \frac{2(m-1)M_1(G) + 2m(\Pi_1^*(G))^{\frac{1}{m}}}{H(G)} + \frac{H(G)\left(\Delta_e^{3/2} - \delta_e^{3/2}\right)^2}{8}. \tag{14}$$

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

Corollary 3.2. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$\begin{aligned} HM(G) \leq & \frac{2m(m-1)(\Delta_e+\delta_e) + 2m(\Pi_1^*(G))^{\frac{1}{m}}}{H(G)} + \\ & + \frac{H(G)\left(\Delta_e^{3/2} - \delta_e^{3/2}\right)^2 - 8(m-1)\Delta_e\delta_e}{8}. \end{aligned} \tag{15}$$

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

Proof. For $p_i = \frac{1}{m}$, $a_i = d(e_i)+2$, $r = \delta_e$, $R = \Delta_e$, $i = 1, 2, \ldots, m$, the inequality (8) becomes

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

i.e.

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

From the above and (14) we arrive at (15). □

In the following theorem we establish an upper bound for $HM(G)$ in terms of parameter m and invariants $M_1(G)$ and $\Pi_1^*(G)$.

Theorem 3.2. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$HM(G) \leq M_1(G)^2 - m(m-1)(\Pi_1^*(G))^{\frac{2}{m}}. \tag{16}$$

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

Proof. Setting $a_i = (d(e_i)+2)^2$, $i = 1, 2, \ldots, m$, in (7) we get

$$\left(\sum_{i=1}^{m}(d(e_i)+2)\right)^2 \geq \sum_{i=1}^{m}(d(e_i)+2)^2 + m(m-1)\left(\prod_{i=1}^{m}(d(e_i)+2)^2\right)^{\frac{1}{m}}, \tag{17}$$

i.e.

$$M_1(G)^2 \geq HM(G) + m(m-1)(\Pi_1^*(G))^{\frac{2}{m}}.$$

According to the above we obtain (16).

Equality in (7) holds if and only if $a_1 = a_2 = \cdots = a_m$, therefore equality in (17) holds if and only if $d(e_1)+2 = d(e_2)+2 = \cdots = d(e_m)+2$. Consequently, the equality in (16) holds if and only if $L(G)$ is a regular graph. □

In the next theorem we determine an upper bound for $HM(G)$ in terms of parameters m, Δ_e, δ_e and invariant $M_1(G)$.

Theorem 3.3. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$HM(G) \leq \frac{M_1(G)^2}{m}\left(1+\alpha(S)\frac{(\Delta_e-\delta_e)^2}{\Delta_e\delta_e}\right), \tag{18}$$

where

$$\alpha(S) = \frac{\sum\limits_{i\in S}(d(e_i)+2)}{M_1(G)}\left(1-\frac{\sum\limits_{i\in S}(d(e_i)+2)}{M_1(G)}\right) \tag{19}$$

and S is a subset of $I_m = \{1,2,\ldots,m\}$ which minimizes the expression

$$\left|\sum_{i\in S}(d(e_i)+2)-\frac{1}{2}M_1(G)\right|. \tag{20}$$

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

Proof. For $p_i = d(e_i)+2$, $i=1,2,\ldots,m$, from (2) and (3) we obtain that S is a subset of I_m which minimizes the expression (20) and $\gamma(S) = \alpha(S)$, where $\alpha(S)$ is defined by (19). Further, for $p_i = a_i = d(e_i)+2$, $r = \delta_e$, $R = \Delta_e$, $i = 1,2,\ldots,m$, the inequality (3) becomes

$$m\sum_{i=1}^{m}(d(e_i)+2)^2 \leq \left(1+\alpha(S)\frac{(\Delta_e-\delta_e)^2}{\Delta_e\delta_e}\right)\left(\sum_{i=1}^{m}(d(e_i)+2)\right)^2,$$

i.e.

$$mHM(G) \leq M_1(G)^2\left(1+\alpha(S)\frac{(\Delta_e-\delta_e)^2}{\Delta_e\delta_e}\right), \tag{21}$$

wherefrom (18) follows.

Equality in (3) holds if and only if $R = a_1 = a_2 = \cdots = a_m = r$, therefore equality in (21) holds if and only if $\Delta_e = d(e_1)+2 = d(e_2)+2 = \cdots = d(e_m)+2 = \delta_e$. This means that equality in (18) holds if and only if $L(G)$ is a regular graph. □

Since $\alpha(S) \leq \frac{1}{4}$ for any $S \subset I_m$, we have the following corollary of Theorem 3.3.

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

$$HM(G) \leq \frac{M_1(G)^2}{4m}\left(\sqrt{\frac{\Delta_e}{\delta_e}}+\sqrt{\frac{\delta_e}{\Delta_e}}\right)^2. \tag{22}$$

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

Remark 3.1. *Since $2\delta \leq \delta_e \leq \Delta_e \leq 2\Delta$, from (22) the inequality*

$$HM(G) \leq \frac{M_1(G)^2}{4m}\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)^2$$

is obtained, which was proven in [12]. The equality holds if and only if G is regular.

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