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A Short Note On Hyper Zagreb Index

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abstract: In this paper, we present and analyze the upper and lower bounds on the Hyper-Zagreb index $\chi^2(G)$ of graph G in terms of the number of vertices (n), number of edges (m), maximum degree (Δ), minimum degree (δ) and the inverse degree ($ID(G)$). In addition, a counter example on the upper bound of the second Zagreb index for Theorems 2.2 and 2.4 from [20] is provided. Finally, we present the lower and upper bounds on $\chi^2(G) + \chi^2(\overline{G})$, where $\overline{G}$ denotes the complement of G.

Key Words: First Zagreb index, Second Zagreb index, Hyper Zagreb index.

Contents

1. Introduction

Let G be a simple graph with the vertex set $V(G)$ and the edge set $E(G)$. As usual, we denote the degree of a vertex by $d_i = d(v_i)$ for $i = 1, 2, \ldots, n$ such that $d_1 \geq d_2 \geq \cdots \geq d_n$, with the maximum, second maximum and the minimum vertex degree of G are denoted by $\Delta = \Delta(G)$, $\Delta_2 = \Delta_2(G)$ and $\delta = \delta(G)$ respectively. $\overline{G}$ denotes the complement of G, with the same vertex set such that two vertices u and v are adjacent in $\overline{G}$ if and only if they are not adjacent in G. A *line graph* $L(G)$ obtained from G in which $V(L(G)) = E(G)$, where two vertices of $L(G)$ are adjacent if and only if they are adjacent edges of G.

In 1972, the *first and second Zagreb indices* are introduced by Gutman and Trinajstić [13,14] and are defined as

$$M_1^2(G) = \sum_{v \in V(G)} d(v)^2 \quad \text{and} \quad M_2^1(G) = \sum_{uv \in E(G)} d(u)d(v).$$

In 1987, the *inverse degree* first attracted attention through conjectures of the computer program Graffiti [11]. The inverse degree of a graph G with no isolated vertices are defined as

$$ID(G) = \sum_{u \in V(G)} \frac{1}{d(u)}.$$

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In 2005, Li and Zheng [15] introduced the generalized version of the first Zagreb index. For $\alpha \in \mathbb{R}$ and G be any graph which satisfies the important identity (1.1)

$$M_1^{\alpha+1}(G) = \sum_{v\in V(G)} d(v)^{\alpha+1} = \sum_{uv\in E(G)} [d(u)^{\alpha} + d(v)^{\alpha}]. \tag{1.1}$$

In 2010, Ashrafi, Došlić and Hamzeha introduced the concept of sum of non-adjacent vertex degree pairs of the graph G, known as *first and second Zagreb coindices* [2] and are defined as

$$\overline{M}_1^2 = \overline{M}_1^2(G) = \sum_{uv\notin E(G)} [d(u) + d(v)] \quad \text{and} \quad \overline{M}_2^1 = \overline{M}_2^1(G) = \sum_{uv\notin E(G)} d(u)d(v).$$

In 2013, Shirdel, Rezapour, and Sayadi [16] defined the *Hyper-Zagreb index* as

$$HM(G) = \sum_{uv\in E(G)} [d(u) + d(v)]^2. \tag{1.2}$$

In 2015, Fortula and Gutman [12,13] introduced the *forgotten topological index* and for $\alpha = 2$ in (1.1) turns it as a very special case formula, defined by

$$M_1^3(G) = \sum_{v\in V(G)} d(v)^3 = \sum_{uv\in E(G)} \left[d(u)^2 + d(v)^2\right].$$

As usual $P_n, K_{1,n-1}, C_n, K_n$ denotes the *path, star, cycle and complete graphs* on n vertices respectively. The *wheel graph* W_n is join of the graphs C_{n-1} and K_1. Bidegreed graph is a graph whose vertices have exactly two vertex degrees Δ and δ. The *Helm graph* H_n is obtained from W_n by adjoining a pendant edge at each vertex of the cycle. Let G and H be any graph. Then $\sigma_G(H)$ represents the total number of distinct subgraphs of the graph G which are isomorphic to H. The *tensor product of the two simple graphs* G and H are denoted by $G \times H$, whose vertex set is $V(G) \times V(H)$ in which (g_1, h_1) and (g_2, h_2) are adjacent whenever g_1g_2 is an edge in G and h_1h_2 is an edge in H.

For computational purposes, we use the software GraphTea [1] considering various phases of testing. GraphTea is a graph visualization software designed specifically to visualize and explore graph algorithms and topological indices interactively.

2. Upper bounds for $\chi^2(G)$

An equivalent formula for the Hyper-Zagreb index was already in use, pertaining to the first and second Zagreb index. In 2010, Zhou and Trinajstić [21] proposed the general *sum-connectivity index* defined as

$$\chi^{\alpha} = \chi^{\alpha}(G) = \sum_{uv\in E(G)} [d(u) + d(v)]^{\alpha}. \tag{2.1}$$

Obviously, $\chi^0(G) = m, \chi^1(G) = M_1^2(G)$. For $\alpha = 2$, in (2.1) turns the Hyper-Zagreb index as its special case. At first we give the identity for the Hyper-Zagreb index.

Lemma 2.1. *Let G be any simple graph, then*

$$\chi^2(G) = 6\sigma_G(K_{1,3}) + 2\sigma_G(P_4) + 10\sigma_G(P_3) + 6\sigma_G(C_3) + 6m. \tag{2.2}$$

Proof. By the definition of the general sum-connectivity index and using (1.1), we get

$$\chi^2(G) = \sum_{u \in V(G)} d(u)^3 + 2 \sum_{uv \in E(G)} d(u)d(v). \tag{2.3}$$

Thus, by using $M_1^2(G), M_1^3(G)$ and $M_2^1(G)$ from [4], we complete the proof. □

It is easy to see that, an upper bound for either $M_2^1(G)$ or $M_1^3(G)$ suits for $\chi^2(G)$. In the preparations of presenting the upper bounds for $\chi^2(G)$ through the existing upper bounds for the second Zagreb index, we encountered the following upper bounds

Theorem 2.2. [20] *For a simple connected graph G,*

$$M_2^1(G) \le 2\Delta m. \tag{2.4}$$

Theorem 2.3. [20] *For a simple connected graph G,*

$$M_2^1(G) \le \Delta n(n-1) - \overline{M_1^2(G)}. \tag{2.5}$$

Remark 2.4. Counterexamples for the above two theorems. *For any edge $uv \in E(G)$, it is clear that $d(u)d(v) \le d(u)\Delta$. But $\sum_{uv \in E(G)} d(u) \le \sum_{u \in V(G)} d(u)$ need not be true for all graphs. For $K_{1,3}$, $\sum_{u \in V(G)} d(u) = 6$, and for $\sum_{uv \in E(G)} d(u)$ we have the following combinations $3, 5, 7, 9$. Therefore Inequality (2.4) is not true in general. In addition, for the helm H_3 (See Figure 1) with $\Delta = 4$ and second Zagreb index is 96, but the $2\Delta m$ is 72.*

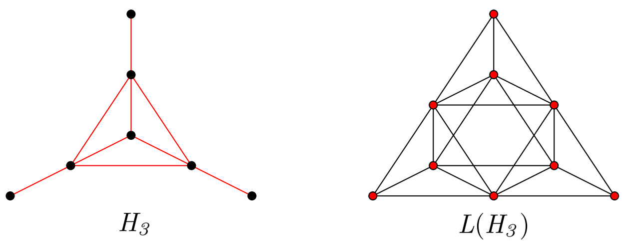

Figure 1: The Helm H_3 and its Line graph $L(H_3)$.

In analogy, Inequality (2.5) is also not true in general. By considering $L(H_3)$ with the first Zagreb coindex is 126 and $\Delta n(n-1) - \overline{M_1^2(G)}$ is 306, but the second

Zagreb index of $L(H_3)$ is 516. Let $\sum[d(u)+d(v)]$ denote the total number of combinations of sum of the vertices u, v in G and is represented as

$$\sum[d(u)+d(v)] = \sum_{uv\in E(G)}[d(u)+d(v)] + \sum_{uv\notin E(G)}[d(u)+d(v)].$$

For any simple graph G with $\delta \geq 2$ then, it is easy to see that $d(u)+d(v) \leq d(u)d(v)$ for all $uv \in E(G)$. By adding over all the edges, we have $M_1^2(G) \leq M_2^1(G)$, utilizing the result we get $M_2^1(G) \geq \sum[d(u)+d(v)] - \overline{M_1^2(G)}$, but this inequality is mentioned in the Theorem 2.4 of [20] in reverse order, which leads to the counterexample in Figure 1.

Note that forgotten topological index [12] has only few lower bounds. At first, we give an upper bound for $M_1^3(G)$ which leads to the upper bound for $\chi^2(G)$.

Theorem 2.5. *Let G be any simple graph with no isolated vertices. Then*

$$\chi^2(G) \leq 2M_2^1(G) + (\Delta+\delta)\left(M_1^2(G)-n\right) + 2m - \Delta\delta\,(2m - ID(G)) \tag{2.6}$$

equality if and only if G is regular or bidegreed graph.

Proof. Let $a, A \in \mathbb{R}$ and x_i, y_i be two sequences with the property $ay_i \leq x_i \leq Ay_i$ for $i = 1, 2, \dots, n$ and w_i be any sequence of positive real numbers, it holds $w_i\,(Ay_i - x_i)\,(x_i - ay_i) \geq 0$. Since w_i is a positive sequence, choose $w_i = m_i - n_i$ such that $m_i \geq n_i$. we get

$$\sum_{i=1}^{n}(m_i - n_i)\left[(A+a)x_iy_i - x_i^2 - Aay_i^2\right] \geq 0 \tag{2.7}$$

By setting $A = \Delta$, $a = \delta$, $x_i = d(v_i)$, $y_i = 1$, $m_i = d(v_i)$ and $n_i = d(v_i)^{-1}$, we obtain

$$(\Delta+\delta)\sum_{i=1}^{n} d(v_i)^2 - \sum_{i=1}^{n} d(v_i)^3 - \Delta\delta\sum_{i=1}^{n} d(v_i) \geq (\Delta+\delta)\sum_{i=1}^{n} 1 - \sum_{i=1}^{n} d(v_i) - \Delta\delta\sum_{i=1}^{n}\frac{1}{d(v_i)}$$
$$(\Delta+\delta)\,M_1^2(G) - M_1^3(G) - 2m\Delta\delta \geq (\Delta+\delta)\,n - 2m - \Delta\delta ID(G).$$

Substituting the above inequality into (2.1) completes the proof and the equality holds if and only if G is regular. □

Theorem 2.6. *Let G be any simple graph with n vertices and m edges. Then*

$$\chi^2(G) \leq 2M_2^1(G) + (\Delta+\delta+1)\,M_1^2(G) - (2m - n\Delta)\delta - 2m\Delta\,(\delta+1) \tag{2.8}$$

equality if and only if G is regular or bidegreed graph.

Proof. The proof follows by using similar arguments as in the proof of Theorem 2.5 with setting $m_i = d(v_i)$ and $n_i = 1$. □

Remark 2.7. *The upper bounds* (2.6) *and* (2.8) *are incomparable. For the graphs* H_3 *and* $L(H_3)$ *depicted in Figure 1,* (2.6) *is better than* (2.8) *and for the graphs* $H_3 \times H_3, H_3 \times L(H_3)$ *and* $L(H_3) \times L(H_3)$, (2.8) *is better than* (2.6)*, as shown in the next table*

	H_3	$L(H_3)$	$H_3 \times H_3$	$H_3 \times L(H_3)$	$L(H_3) \times L(H_3)$
n	7	9	49	63	81
m	9	21	162	378	882
$\chi^2(G)$	414.0	2136	86148.0	443232.0	2283840.0
(2.6)	419.333	2767.8	145902.778	746861.4	3666048.84
(2.8)	418.0	2790.0	145756.0	745236.0	3659652.0

3. Lower bounds for $\chi^2(G)$

Zhou and Trinajstić [21] obtained the following lower bound for $\chi^2(G)$.

Theorem 3.1. [21] *Let* G *be a simple graph* G *with* $m \geq 1$ *edges. Then*

$$\chi^2(G) \geq \frac{M_1^2(G)^2}{m} \tag{3.1}$$

equality holds if and only if $d(u) + d(v)$ *is a constant for any edge* uv.

Theorem 3.2. *Let* G *be a simple graph with* n *vertices and* m *edges, then*

$$\chi^2(G) \geq 4M_2^1(G) \tag{3.2}$$

equality holds if and only if G *is regular.*

Proof. For any two non-negative real numbers a, b we have $\frac{1}{4}(a+b)^2 \geq ab$. Thus, by fixing $a = d(u)$ and $b = d(v)$ for $uv \in E(G)$, then adding over all the edges of G yields

$$\frac{1}{4} \sum_{uv \in E(G)} (d(u) + d(v))^2 \geq \sum_{uv \in E(G)} d(u)d(v),$$

which completes the proof, and the equality holds if and only if G is regular. □

Theorem 3.3. *Let* G *be a simple graph with no isolated vertices. Then*

$$\chi^2(G) \geq 2M_2^1(G) + \frac{1}{2m}\left(M_1^2(G)^2 + 2mID(G) - n^2\right) \tag{3.3}$$

equality holds if and only if G *is regular.*

Proof. Consider $w_1, w_2, \ldots, w_n$ be the non-negative weights, then we have the weighted version of Cauchy-Schwartz inequality

$$\sum_{i=1}^{n} w_i a_i^2 \sum_{i=1}^{n} w_i b_i^2 \geq \left(\sum_{i=1}^{n} w_i a_i b_i\right)^2.$$

Since w_i is non-negative, we assume that $w_i = m_i - n_i$ such that $m_i \geq n_i \geq 0$. Thus

$$\sum_{i=1}^{n} m_i a_i^2 \sum_{i=1}^{n} m_i b_i^2 - \left(\sum_{i=1}^{n} m_i a_i b_i\right)^2 \geq \sum_{i=1}^{n} n_i a_i^2 \sum_{i=1}^{n} n_i b_i^2 - \left(\sum_{i=1}^{n} n_i a_i b_i\right)^2 \geq 0. \tag{3.4}$$

Set $m_i = d(v_i)$, $n_i = \frac{1}{d(v_i)}$, $a_i = d(v_i)$ and $b_i = 1$, for all $i = 1, 2, \cdots, n$ in the above, we get

$$\sum_{i=1}^{n} d(v_i)^3 \sum_{i=1}^{n} d(v_i) - \left(\sum_{i=1}^{n} d(v_i)^2\right)^2 \geq \sum_{i=1}^{n} d(v_i) \sum_{i=1}^{n} \frac{1}{d(v_i)} - \left(\sum_{i=1}^{n} 1\right)^2.$$

By combining the above inequality with (2.1), we complete the proof and the equality holds if and only if G is regular. □

Theorem 3.4. *Let G be a simple graph with n vertices and m edges, then*

$$\chi^2(G) \geq 2M_2^1(G) + \frac{1}{2m}\left(M_1^2(G)^2 + nM_1^2(G) - 4m^2\right) \tag{3.5}$$

equality holds if and only if G is regular.

Proof. The proof follows from the same terminology of Theorem 3.4 by choosing $m_i = d(v_i)$, $n_i = 1$, $a_i = d(v_i)$ and $b_i = 1$, for all $i = 1, 2, \cdots, n$. □

Remark 3.5. *For every simple graph G, the lower bound in (3.5) is always better than the lower bound in (3.3). For this, we have to show that*

$$nM_1^2(G) - 4m^2 \geq 2mID(G) - n^2 \tag{3.6}$$

by fixing $a_i = d(v_i)$, $b_i = 1, m_i = 1$ and $n_i = d(v_i)^{-1}$ in (3.4), we achieve our required claim.

Remark 3.6. *The lower bounds in (3.1), (3.2) and (3.3) are not comparable.*

	H_4	$L(H_4)$	$L(L(H_4))$
$\chi^2(G)$	612	3564	43764
(3.1)	588	3499.2	43201.09
(3.2)	576	3456	43296
(3.3)	583.875	3477.867	43248.65
(3.5)	589.5	3482.4	43255.91

In [21], the following lower and upper bound for $\chi^2(G)+\chi^2(\overline{G})$ was established:

$$\frac{n(n-1)^3}{2} \leq \chi^2(G) + \chi^2(\overline{G}) \leq 2n(n-1)^3$$

By using Theorems 2.5 and 3.4, we deduce a finer bound for $\chi^2(G) + \chi^2(\overline{G})$.

Theorem 3.7. *Let G be a graph of order n with m edges. Then*

$$(i)\ \chi^2(G) + \chi^2(\overline{G}) \leq 2n(n-1)^3 - 12m(n-1)^2 + 4m^2 + (5n-6)\left[(\Delta+\delta)(2m-n) + 2m - \Delta\delta(n - ID(G))\right]$$

equality holds if and only if G is regular.

$$(ii)\ \chi^2(G) + \chi^2(\overline{G}) \geq 2n(n-1)^3 - 12m(n-1)^2 + 4m^2 + \frac{(5n-6)}{n}\left[2mID(G) + 4m^2 - n^2\right]$$

equality holds if and only if G is regular.

Proof. One of the present author with Song [17] have established the following identity

$$M_1^3(G) + M_1^3(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1^2(G).$$

From [7], we have

$$M_2^1(G) + M_2^1(\overline{G}) = \frac{n(n-1)^3}{2} - 3m(n-1)^2 + 2m^2 + \left(n - \frac{3}{2}\right)M_1^2(G).$$

By using the above results in Lemma 2.1, we get

$$\chi^2(G) + \chi^2(\overline{G}) = 2n(n-1)^3 - 12m(n-1)^2 + 4m^2 + (5n-6)M_1^2(G).$$

By setting $A = \Delta, a = \delta$, $x_i = d(v_i)$, $y_i = m_i = 1$ and $n_i = d(v_i)^{-1}$ in (2.7) and using (3.6) in the above relation, we get the required result. □

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