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 \( (\Delta) \), minimum degree \( (\delta) \) and the inverse degree \( (\text{ID}(G)) \). 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.

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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

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

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

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

$$M^{\alpha+1}_1(G) = \sum_{v \in V(G)} d(v)^{\alpha+1} = \sum_{uv \in E(G)} [d(u)^{\alpha} + d(v)^{\alpha}]. \quad (1.1)$$

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

$$M^2_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

and

$$M^1_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

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

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

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

$$M^3_1(G) = \sum_{v \in V(G)} d(v)^3 = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2].$$

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 $\Delta$ and $\delta$. 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

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

Obviously, $\chi^0(G) = m, \chi^1(G) = M^2_1(G)$. 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

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

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

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

Thus, by using $M^2_1(G), M^3_1(G)$ and $M^1_2(G)$ from [4], we complete the proof. \qed

It is easy to see that, an upper bound for either $M^2_1(G)$ or $M^3_1(G)$ 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 $G$,

$$
M^1_2(G) \leq 2\Delta m. \quad (2.4)
$$

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

$$
M^1_2(G) \leq \Delta n(n-1) - M^3_1(G). \quad (2.5)
$$

Remark 2.4. Counterexamples for the above two theorems. For any edge $uv \in E(G)$, it is clear that $d(u)d(v) \leq d(u)\Delta$. But $\sum_{uv \in E(G)} d(u) \leq \sum_{u \in V(G)} d(u)$ 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 $L(H_3)$.](image)

In analogy, Inequality (2.5) is also not true in general. By considering $L(H_3)$ with the first Zagreb coindex is 126 and $\Delta n(n-1) - M^3_1(G)$ is 306, but the second
Proof. The proof follows by using similar arguments as in the proof of Theorem 2.6.

Let \(G\) be any simple graph with no isolated vertices. Then

\[
\chi^2(G) \leq 2M_2^1(G) + (\Delta + \delta) (M_2^2(G) - n) + 2m - \Delta \delta (2m - ID(G))
\] (2.6)

equality if and only if \(G\) is regular or bidegreed graph.

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

\[
\chi^2(G) \leq 2M_2^1(G) + (\Delta + \delta) (M_2^2(G) - n) + 2m - \Delta \delta (2m - ID(G))
\] (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 \(ax_i \leq x_i \leq Ay_i\) for \(i = 1, 2, \ldots, n\) 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

\[
\sum_{i=1}^{n} (m_i - n_i) [(A + a)x_i y_i - x_i^2 - Ay_i^2] \geq 0
\] (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

\[
(\Delta + \delta) \sum_{i=1}^{n} d(v_i) - \Delta \delta \sum_{i=1}^{n} d(v_i) \geq (\Delta + \delta) \sum_{i=1}^{n} 1 - \sum_{i=1}^{n} d(v_i) - \Delta \delta \sum_{i=1}^{n} \frac{1}{d(v_i)}
\]

\[
(\Delta + \delta) M_2^2(G) - M_2^1(G) - 2m \Delta \delta \geq (\Delta + \delta) n - 2m - \Delta \delta ID(G).
\]

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

\[
\chi^2(G) \leq 2M_2^1(G) + (\Delta + \delta + 1) M_2^2(G) - (2m - n\Delta)\delta - 2m\Delta (\delta + 1)
\] (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.

<table>
<thead>
<tr>
<th></th>
<th>$H_3$</th>
<th>$L(H_3)$</th>
<th>$H_3 \times H_3$</th>
<th>$H_3 \times L(H_3)$</th>
<th>$L(H_3) \times L(H_3)$</th>
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<td>9</td>
<td>49</td>
<td>63</td>
<td>81</td>
</tr>
<tr>
<td>$m$</td>
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<td>21</td>
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<td>882</td>
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<td>86148.0</td>
<td>443232.0</td>
<td>2283840.0</td>
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<td>419.333</td>
<td>2767.8</td>
<td>145902.778</td>
<td>746861.4</td>
</tr>
<tr>
<td></td>
<td>(2.8)</td>
<td>418.0</td>
<td>2790.0</td>
<td>145756.0</td>
<td>745236.0</td>
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</tbody>
</table>

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

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

(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

$$\chi^2(G) \geq 4M_1^2(G)$$

(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. \(\Box\)

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

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

(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

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

(3.4)

Set \( m_i = d(v_i) \), \( n_i = 1/d(v_i) \), \( a_i = d(v_i) \) and \( b_i = 1 \), for all \( i = 1, 2, \ldots, n \) 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. \( \square \)

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

\[
\chi^2(G) \geq 2M^1_1(G) + \frac{1}{2m} \left( M^2_1(G)^2 + nM^2_1(G) - 4m^2 \right)
\]

(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 \( i = 1, 2, \ldots, n \). \( \square \)

**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

\[
nM^2_1(G) - 4m^2 \geq 2mID(G) - n^2
\]

(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.

<table>
<thead>
<tr>
<th>( \chi^2(G) )</th>
<th>( L(H_4) )</th>
<th>( L(L(H_4)) )</th>
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<td>(3.1) 588</td>
<td>3499.2</td>
<td>43201.09</td>
</tr>
<tr>
<td>(3.2) 576</td>
<td>3456</td>
<td>43296</td>
</tr>
<tr>
<td>(3.3) 583.875</td>
<td>3477.867</td>
<td>43248.65</td>
</tr>
<tr>
<td>(3.5) 589.5</td>
<td>3482.4</td>
<td>43255.91</td>
</tr>
</tbody>
</table>

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

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

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

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

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

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. \qed

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