

BOUNDS OF ZAGREB INDICES AND HYPER ZAGREB INDICES

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The hyper Zagreb index is a kind of extensions of Zagreb indices, used for predicting physicochemical properties of organic compounds. Given a graph $G = (V(G), E(G))$, the first hyper-Zagreb index is the sum of the square of edge degree over edge set $E(G)$ and defined as $HM_1(G) = \sum_{e=uv \in E(G)} d(e)^2$, where $d(e) = d(u) + d(v)$ is the edge degree. In this work, we define the second hyper-Zagreb index on the adjacent edges as $HM_2(G) = \sum_{e \sim f} d(e)d(f)$, where $e \sim f$ represents the adjacent edges of G . By inequalities, we explore some upper and lower bounds of these hyper-Zagreb indices, and provide the relation between Zagreb indices and hyper Zagreb indices.

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1. INTRODUCTION

The graphs $G = (V(G), E(G))$ considered in this paper are finite, loopless and contain no multiple edges. Given a graph $G = (V, E)$, V and E represent the set of vertices and the set of edges with $n = |V|$ vertices and $m = |E|$ edges, respectively. For a vertex $u \in V$, the number of vertices adjacent with u is called its degree $d(u)$. In a graph G , Δ and δ represent the maximum and the minimum degree, respectively.

In 1947, Harold Wiener introduced famous the Wiener index, a most widely known topological descriptor [31]. The Winner index is the oldest and one of the most popular molecular structure descriptors, well correlated with many physical and chemical properties of a variety of classes of chemical compounds. Based on the success on the Wiener index, many topological indices have been introduced. Almost forty years ago, Gutman *et al.* defined the important degree-based topological indices: the first and second Zagreb indices [10]. These are defined as

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

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In 2004, Miličević [19] reformulated these Zagreb indices in terms of edge degrees, $d(e) = d(u) + d(v) - 2$, for $e = uv$ and defined reformulated Zagreb indices,

$$EM_1(G) = \sum_{e \in E(G)} d(e)^2, EM_2(G) = \sum_{e \sim f} d(e)d(f).$$

In 2013, Shirdel *et al.* [24] defined the *first hyper Zagreb index* as follows,

$$HM_1(G) = \sum_{e \in E(G)} d(e)^2,$$

where $d(e) = d(u) + d(v)$. In 2016, Jamil *et al.* [8] improved and extended Shirdel's results. Based on this definition of edge degree, we define the *second hyper Zagreb index* as follows,

$$HM_2(G) = \sum_{e \sim f} d(e)d(f),$$

where $e \sim f$ represents the adjacent edges of G . Furthermore, G is called regular if every vertex has the same degree and edge degree regular if every edge has the same degree, respectively.

These graph invariants, based on vertex-degrees and edge-degrees of a graph, are widely used in theoretical chemistry. For applications of Zagreb indices in QSPR/QSAR and latest results, refer to [1–3, 6, 7, 9, 12–17, 21, 22, 25–30, 32].

As a fundamental dynamical processing system, the basis of graph structure has received considerable interest from the scientific community. Recent work shows that the key quantity-degree-based topological indices to a given graph class on uncorrelated random scale-free networks is qualitatively reliant on the heterogeneity of network structure. However, in addition to the transformations of these graph basis, most real system models (topological indices) are also characterized by degree correlations. In this paper, we explore some properties of hyper Zagreb indices in terms of the number of vertices n , the number of edges m , maximum and minimum degree Δ, δ , respectively. Also we provide the relation between hyper Zagreb indices and first Zagreb index $M_1(G)$.

2. PRELIMINARIES AND MAIN RESULTS

After introducing the construction and structural properties of degree-based topological indices, we will provide our main results by presenting their inequalities.

THEOREM 1. *Let G be a graph with n number of vertices and m number of edges, then*

$$\delta^2 \leq \frac{HM_1(G)}{4m} \leq \Delta^2,$$

the left and right equalities hold if and only if G is δ -regular and Δ -regular, respectively.

Proof. Note that $\delta \leq d(v_i) \leq \Delta$, $i = 1, 2, \dots, n$. Then

$$2\delta \leq d(e_j) \leq 2\Delta, \quad j = 1, 2, \dots, m.$$

By the definition of the first hyper Zagreb index, we have

$$\delta^2 \leq \frac{HM_1(G)}{4m} \leq \Delta^2.$$

Clearly, the equalities hold if and only if G is δ -regular and Δ -regular. In particular, if G is general regular connected graph, then $\delta(G) = 2$ and $\Delta(G) = n - 1$. \square

THEOREM 2. *Let G be a graph with m edges, then*

$$HM_1(G) \geq \frac{M_1(G)^2}{m},$$

the equality holds if and only if G is edge degree regular.

Proof. Let $d(e_i)$ be the edge degree of G . By Cauchy-Schwartz inequality, we obtain

$$\begin{aligned} [d(e_1)^2 + d(e_2)^2 + \dots + d(e_m)^2][1^2 + 1^2 + \dots + 1^2] \\ \geq [d(e_1) \cdot 1 + d(e_2) \cdot 1 + \dots + d(e_m) \cdot 1]^2. \end{aligned}$$

Note that $\sum_{e \in E(G)} d(e) = \sum_{v \in V(G)} d(v)^2$. By the concept of $M_1(G)$, we obtain the relation between $HM_1(G)$ and $M_1(G)$ below.

$$HM_1(G) \cdot m \geq M_1(G)^2,$$

that is,

$$HM_1(G) \geq \frac{M_1(G)^2}{m}.$$

Clearly, the equality holds if and only if every edge has the same degree, that is, G is edge degree regular. \square

THEOREM 3. *Let G be a graph with n vertices and m edges, then*

$$HM_1(G) \leq M_1(G)(m + 2\delta - 1) - 2m(m - 1)\delta,$$

the equality holds if and only if G is regular.

Proof. We keep the same notations as [5]. Let $d(e_i)\mu_i$ be the sum of degrees of the edges adjacent to the edge e_i . We have

$$d(e_i)\mu_i = \sum_{e_i \sim e_j} d(e_j) \leq \sum_{i=1}^m d(e_i) - d(e_i) - (m - 1 - d(e_i))2\delta.$$

Thus,

$$\begin{aligned} HM_1(G) &= \sum_{e_i \in E(G)} d(e_i)^2 = \sum_{i=1}^m d(e_i)\mu_i \\ &\leq \sum_{i=1}^m [\sum_{i=1}^m d(e_i) - d(e_i) - (m - d(e_i))2\delta] \\ &= M_1(G)(m + 2\delta - 1) - 2m(m - 1)\delta. \end{aligned}$$

Clearly, the equality holds if and only if G is regular. \square

By the results of [11] that $M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta$, where the equality holds if and only if G is regular, we have the following corollary.

COROLLARY 1. *Let G be a graph with n vertices and m edges, then*

$$HM_1(G) \leq (2m(\Delta + \delta) - n\Delta\delta)(m + 2\delta - 1) - 2m(m - 1)(\delta - 1),$$

where the equality holds if and only if G is regular.

THEOREM 4. *Let G be a graph with n vertices, m edges and minimum degree $\delta \geq 2$, then*

$$HM_1(G) \leq \frac{(\Delta + \delta)^2}{4m\Delta\delta} M_1(G)^2,$$

the equality holds if and only if G is a regular graph, or there are exactly $\frac{m\delta}{\Delta + \delta}$ edges of degree 2Δ and $\frac{m\Delta}{\Delta + \delta}$ edges of degree 2δ such that $(\Delta + \delta)$ divides $m\delta$.

Proof. If a, a_1, a_2, \dots, a_m and b, b_1, b_2, \dots, b_m are positive real numbers such that $a \leq a_i \leq A, b \leq b_i \leq B$ for $1 \leq i \leq m$ with $a < A$ and $b < B$, by Pólya-Szegő Inequality [20], we have

$$\sum_{i=1}^m a_i^2 \cdot \sum_{i=1}^m b_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}} \right)^2 \cdot \left(\sum_{i=1}^m a_i b_i \right)^2,$$

and the equality holds if and only if the numbers

$$k = \frac{\frac{A}{a}}{\frac{A}{a} + \frac{B}{b}}, l = \frac{\frac{B}{b}}{\frac{A}{a} + \frac{B}{b}}$$

are integers, $a = a_1 = a_2 = \dots = a_k; A = a_{k+1} = a_{k+2} = \dots = a_m$ and $B = b_1 = b_2 = \dots = b_l; b = b_{l+1} = b_{l+2} = \dots = b_m$. If we allow $a = A$ or

$b = B$, the equality holds if $AB = ab$, i.e., $A = a = a_1 = a_2 = \dots = a_m$ and $B = b = b_1 = b_2 = \dots, b_m$. By setting the values $a_i = 1$ and $b_i = d(e_i)$ for $i = 1, 2, \dots, m$, we obtain

$$\sum_{i=1}^m 1^2 \cdot \sum_{i=1}^m d(e_i)^2 \leq \frac{(AB + ab)^2}{4ABab} \cdot \left(\sum_{i=1}^m d(e_i) \right)^2.$$

So,

$$mHM_1(G) \leq \frac{(AB + ab)^2}{4ABab} \cdot M_1(G)^2.$$

Now since $a \leq a_i \leq A$, we have $a = A = 1$ and since $b \leq b_i \leq B$, we have $b = 2\delta$ and $B = 2\Delta$. Hence,

$$HM_1(G) \leq \frac{(2\Delta + 2\delta)^2}{16\Delta\delta} M_1(G)^2,$$

which is the expected result. In the last expression, the equality holds if and only if G is a regular graph, or there are exactly $\frac{m\delta}{\Delta+\delta}$ edges of degree 2Δ and $\frac{m\Delta}{\Delta+\delta}$ edges of degree 2δ such that $(\Delta + \delta)$ divides $m\delta$. \square

COROLLARY 2. *Let G be a graph with n vertices, m edges and minimum degree $\delta \geq 2$, then*

$$HM_1(G) \leq \frac{(n+1)^2}{8m(n-1)} M_1(G)^2,$$

the equality holds if G has exactly $\frac{m}{n-1}$ edges of degree $2(n-2)$ and $\frac{m(n-2)}{n-1}$ edges of degree 2 such that $n-1$ divides m .

Proof. Note that

$$\frac{(\Delta + \delta)^2}{\Delta\delta} = \frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2.$$

By Theorem 4, we have

$$HM_1(G) \leq \left[\frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2 \right] M_1(G)^2.$$

As the function $f(x) = x + \frac{1}{x}$ is increasing for $x \geq 1$, so $\left[\frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2 \right]$ is increasing for $\frac{\Delta}{\delta} \geq 1$. Now for $\delta \geq 2$, $1 \leq \frac{\Delta}{\delta} \leq \frac{n-1}{2}$. So, $\left[\frac{\Delta}{\delta} + \frac{\delta}{\Delta} + 2 \right] \leq \frac{(n+1)^2}{2(n-1)}$. So,

$$HM_1(G) \leq \frac{(n+1)^2}{8m(n-1)} M_1(G)^2,$$

the equality holds if G has exactly $\frac{m}{n-1}$ edges of degree $2(n-2)$ and $\frac{m(n-2)}{n-1}$ edges of degree 2 such that $n-1$ divides m . \square

COROLLARY 3. Let G be a graph with n vertices and m edges, then

$$HM_1(G) \leq \frac{m^3(n+1)^6}{16n^2(n-1)^2},$$

the equality holds if and only if $G \cong K_3$.

Proof. Note that [11] $M_1(G) \leq \frac{m^2(n+1)^2}{2n(n-1)}$, for $\delta \geq 2$ with the equality holding if and only if $G \cong K_3$. Thus, Corollary 2 yields the result. \square

THEOREM 5. Let G be a graph with n vertices and m edges, then

$$HM_1(G) \leq 2(\Delta + \delta)M_1(G) - 4m\Delta\delta,$$

the equality holds if and only if G is a regular graph.

Proof. Suppose a_i, b_i, p and P are real numbers such that $pa_i \leq b_i \leq Pa_i$ for $i = 1, 2, \dots, m$, then we have Diaz-Metcalf inequality [23],

$$\sum_{i=1}^m b_i^2 + pP \sum_{i=1}^m a_i^2 \leq (p + P) \sum_{i=1}^m a_i b_i,$$

and the equality holds if and only if $b_i = pa_i$ or $b_i = Pa_i$ for every $i = 1, 2, \dots, m$. By setting $a_i = 1$ and $b_i = d(e_i)$, for $i = 1, 2, \dots, m$, from the above inequality we obtain

$$\sum_{i=1}^m d(e_i)^2 + 2\Delta \cdot 2\delta \sum_{i=1}^m 1^2 \leq 2(\Delta + \delta) \sum_{i=1}^m d(e_i).$$

and

$$HM_1(G) \leq 2(\Delta + \delta)M_1(G) - 4m\Delta\delta.$$

Thus, the equality holds if and only if G is a regular graph. \square

By the results of [11] we have, $M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta$, with the equality holding if and only if G is regular. So, we have the following result:

COROLLARY 4. Let G be a graph with n vertices and m edges, then

$$HM_1(G) \leq 4m(\Delta + \delta)^2 - \Delta\delta(n + 4m).$$

THEOREM 6. Let G be a graph with n vertices and m edges, then

$$\delta^2 \leq \frac{HM_2(G)}{2(M_1(G) - 2m)} \leq \Delta^2,$$

the equality holds if and only if G is a regular graph.

Proof. The number of pairs of edges which have a common end point is $\sum_{i=1}^n \binom{d_i}{2} = \frac{1}{2}M_1(G) - 2m$. Also, $2\delta \leq d(e_j) \leq 2\Delta$, for $j = 1, 2, \dots, m$. So, from the definition of second hyper Zagreb index, we have

$$4\left(\frac{1}{2}M_1(G) - m\right)\delta^2 \leq HM_2(G) \leq 4\left(\frac{1}{2}M_1(G) - m\right)\Delta^2,$$

and

$$\delta^2 \leq \frac{HM_2(G)}{2(M_1(G) - 2m)} \leq \Delta^2,$$

the equality holds if and only if G is a regular graph. \square

THEOREM 7. *Let G be a graph with n vertices and m edges, then*

$$HM_2(G) \geq \frac{M_1(G)^3}{2m^2},$$

the equality holds if and only if G is regular.

Proof. For arithmetic and geometric mean inequality,

$$\frac{1}{N} \sum_{e_i \sim e_j} d(e_i)d(e_j) \geq \left[\prod_{e_i \sim e_j} d(e_i)d(e_j) \right]^{\frac{1}{N}} = \left[\prod_{i=1}^m d(e_i)^{d(e_i)} \right]^{\frac{1}{N}},$$

where $N = \frac{1}{2}M_1(G)$. Suppose that $L = \prod_{i=1}^m d(e_i)^{d(e_i)}$. Taking natural logarithm on both sides, we obtain

$$\ln L = \sum_{i=1}^m d(e_i) \ln d(e_i) \geq \sum_{i=1}^m d(e_i) \ln \frac{1}{m} \sum_{i=1}^m d(e_i),$$

and

$$L \geq \left(\frac{M_1(G)}{m} \right)^{M_1(G)}.$$

Hence,

$$\begin{aligned} HM_2(G) &\geq N \left[\frac{M_1(G)}{m} \right]^{\frac{M_1(G)}{N}} \\ &= \frac{M_1(G)^3}{2m^2}. \end{aligned}$$

Clearly, the equality holds if and only if G is a regular graph. \square

THEOREM 8. *Let G be a graph with n vertices and m edges, then*

$$HM_2(G) \leq \frac{1}{2}M_1(G)^2 - \delta(m-1)M_1(G) + \left(\delta - \frac{1}{2}\right)HM_1(G),$$

the equality holds if and only if G is regular.

Proof. By the result of Theorem 3, we have

$$d(e_i)\mu_i = \sum_{e_i \sim e_j} d(e_j) \leq \sum_{i=1}^m d(e_i) - d(e_i) - (m - 1 - d(e_i))2\delta.$$

Thus

$$\begin{aligned} HM_2(G) &= \sum_{e_i \sim e_j} d(e_i)d(e_j) = \frac{1}{2} \sum_{i=1}^m d(e_i)^2\mu_i = \frac{1}{2} \sum_{i=1}^m d(e_i) \left(\sum_{e_i \sim e_j} d(e_j) \right) \\ &\leq \frac{1}{2} \sum_{i=1}^m d(e_i) \left(\sum_{i=1}^m d(e_i) - d(e_i) - 2(m - 1 - d(e_i))\delta \right) \\ &= \frac{1}{2}M_1(G)^2 - \frac{1}{2}HM_1(G) - \delta(m - 1)M_1(G) + \delta HM_1(G). \end{aligned}$$

The expected result is obtained from the above proof process.

Clearly, the equality holds when the graph G is regular. \square

COROLLARY 5. *Let G be a graph with n vertices, m edges and δ minimum degree, then*

$$HM_2(G) \leq \frac{1}{2}K^2 - \left(\delta(m - 1) + \left(\delta - \frac{1}{2} \right)(m + 2\delta - 1) \right) K - m(m - 1)(2\delta - 1)\delta,$$

where $K = M_1(G)$ or $K = 2m(\Delta + \delta - 1) - n\Delta\delta$ with the equality if and only if G is regular.

Proof. Using Theorem 3 and Theorem 8, we obtain the expected result with $K = M_1(G)$. Moreover, we have $M_1(G) \leq 2m(\Delta + \delta - 1) + 2m - n\Delta\delta$ [11] with the equality holding if and only if G is regular, so the expected result clearly follows for $K = 2m(\Delta + \delta - 1) - n\Delta\delta$. \square

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