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Lower and Upper Bounds for Hyper-Zagreb Index of Graphs

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Abstract
The topological indices are functions on the graph that do not depend on the labeling of their vertices. They are used by chemists for studying the properties of chemical compounds. Let G be a simple connected graph. The Hyper-Zagreb index of the graph G, $\mathrm{HM(G)}$, is defined as $\mathrm{HM(G)} = \sum_{\mathrm{e=uv\in E(G)}}(\deg_{\mathrm{G}}^{\mathrm{u}} + \deg_{\mathrm{G}}^{\mathrm{v}})^2$,where $\deg_{\mathrm{G}}^{\mathrm{u}}$ and $\deg_{\mathrm{G}}^{\mathrm{v}}$ are the degrees of vertex u and v, respectively. In this paper, we study the Hyper–Zagreb index and give upper and lower bounds for $\mathrm{HM(G)}$.

Keywords: Hyper–Zagreb index, Vertex degree, First and second Zagreb indices.

الحدود السفلى و العليا لمؤشر فرط – زغرب لرسوم البيانية

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الخلاصة
المؤشرات الطوبوغرافيه هى توابع على الرسم البيانى التى لا تعتمد على وضع العلامات على رؤوسهم. موشرات الطوبوغرافيه تستخدم لخصائص المكونات الكيميائيه مع الكيميائين. عندما يكون G يكون رسم بيانى متصل عادى. الموشر فرط – زغرب من الرسم البيانى G ، HM(G) يعرف ب $\mathrm{HM(G)} = \sum_{\mathrm{e=uv\in E(G)}}(\deg_{\mathrm{G}}^{\mathrm{u}} + \deg_{\mathrm{G}}^{\mathrm{v}})^2$ حيث $\deg_{\mathrm{G}}^{\mathrm{v}}$ $\deg_{\mathrm{G}}^{\mathrm{u}}$ و هى درجات قمه راس u و v على التوالى. في هذا المقاله، ندرس موشر فرط – زغرب و اعطاء الحدود العليا و السفلى لل HM(G).

1. Introduction

Let $G = (V, E)$ be a connected simple graph with vertices set $V(G)$ and edges set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. For a graph G, the degree of vertex $u \in V(G)$ is the number of edges incident to u, denoted as deg_G^u. Moreover, the maximum degree of vertices in graph G is denoted by Δ. A topological index $T(G)$ of a graph G is a number with this property that, for every graph H isomorphic to G, we have

$$T(G) = T(H)$$

The topological indices are functions on the graph that do not depend on the labeling of their vertices. In the definition of the topological indices, there are two vertex-degree based indices, namely the first b index and the second Zagreb index. They are among the oldest and most used molecular structure-descriptors. These Zagreb indices were first introduced by Gutman and Trinajestić [12]. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as follows:

$$M_1(G) = \sum_{v_i \in V(G)} \left(deg_G^{v_i}\right)^2$$

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$$M_2(G)=\sum_{e=uv\in E(G)} deg_G^u.deg_G^v$$

For details of the mathematical properties, bounds, and chemical applications of the Zagreb indices, refer to earlier studies [1- 7, 9-11, 14-18] and for comparing Zagreb indices, refer to other articles [4, 13-16].

In 2013, Shirdel *et al.* [19] introduced a new distance-based Zagreb index named Hyper-Zagreb index, as follows:

$$HM(G)=\sum_{e=uv\in E(G)} (deg_G^u+deg_G^v)^2$$

They computed the Hyper-Zagreb of the Cartesian product, composition, join, and corona product [19]. In 2015, Farahani [8] determined the exact formula of the Hyper-Zagreb index of the Nanotubes $TUSC_4C_8(S)$, as follows:

$$HM(TUSC_4C_8)=12m(36n+5)$$

2. Primary

Consider that $N_G(u)$ denotes the neighbor of u for each $u\in V(G)$. A graph G is r-regular if every vertex of G has a degree r, i.e. all the vertices of G have the same number of neighbors.

Lemma 1. Let G be a connected graph. If $e\notin E(G)$, then

$$HM(G+e)>HM(G)$$

Proof. The proof follows form the definition of the Hyper-Zagreb index ∎ .

Definition 1. The coalescence of G and H is denoted by $G(u)\circ H(v)$ and obtained by identifying the vertex u of G with the vertex v of H.

Theorem 1. Let $P_s=u_1u_2\ldots u_s$, $P_t=v_sv_{s+1}\ldots v_{s+t-1}$ and $P_{s+t-1}=u_1u_2\ldots u_sv_sv_{s+1}\ldots v_{s+t-1}$ be three paths on s,t and $s+t-1$ vertices. Let u be a vertex of graph G. Consider $G_1=\big(G(u)\circ P_s(u_1)\big)(u)\circ P_t(v_s)$ and $G_2=G(u)\circ P_{s+t-1}(u_1)$, then

$$HM(G_1)>HM(G_2)$$

, where G_1 and G_2 are shown in Figure-1.

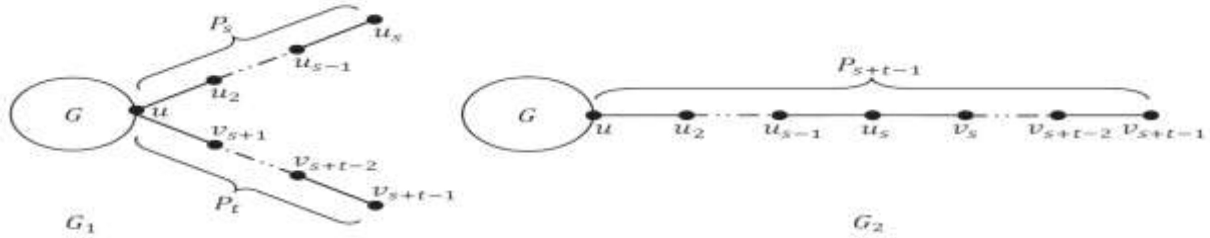

Figure 1- The graphs G_1 and G_2.

Proof. At first, note that in graph G_1 we assume that $u=u_1=v_s$ and in graph G_2, $u=u_1$. Let $E_1=E(G)-\{xu: x\in N_G(u)\}$. Without loss of generality, suppose that $s\geq t$. We assume three cases as follows:

[i] $s,t\neq 2$, In this case, we have

$$\begin{aligned}HM(G_1)=&\sum_{xy\in E_1}\left(deg_{G_1}^x+deg_{G_1}^y\right)^2+\sum_{x\in N_G(u)}\left(deg_{G_1}^u+deg_G^x\right)^2+\left(deg_{G_1}^u+\underbrace{deg_{G_1}^{u_2}}_{2}\right)^2\\&+\left(deg_{G_1}^u+\underbrace{deg_{G_1}^{v_{s+1}}}_{2}\right)^2+\sum_{i=2}^{s-2}\left(\underbrace{deg_{G_1}^{u_i}+deg_{G_1}^{u_{i+1}}}_{4}\right)^2+\left(\underbrace{deg_{G_1}^{u_{s-1}}+deg_{G_1}^{u_s}}_{3}\right)^2\\&+\sum_{i=s+1}^{s+t-3}\left(\underbrace{deg_{G_1}^{v_i}+deg_{G_1}^{v_{i+1}}}_{4}\right)^2+\left(\underbrace{deg_{G_1}^{v_{s+t-2}}+deg_{G_1}^{v_{s+t-1}}}_{3}\right)^2\\=&\sum_{xy\in E_1}\left(deg_G^x+deg_G^y\right)^2+\sum_{x\in N_G(u)}\left(deg_{G_1}^u+deg_G^x\right)^2+2\left(deg_{G_1}^u+2\right)^2+16s\\&+16t-78.\end{aligned}$$

Moreover,

$$HM(G_2) = \sum_{xy\in E_1}\left(deg_{G_2}^{x} + deg_{G_2}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_2}^{u} + deg_{G}^{x}\right)^2 + \left(deg_{G_2}^{u} + deg_{G_2}^{u_2}\right)^2 + 16(s+t-4) + 9.$$

Similarly, since $deg_{G_2}^{u_2} = 2$, $deg_{G_2}^{u} = deg_{G_1}^{u} - 1$, then

$$HM(G_2) = \sum_{xy\in E_1}\left(deg_{G}^{x} + deg_{G}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x} - 1\right)^2 + \left(deg_{G_1}^{u} + 2\right)^2 + 16s + 16t - 55.$$

Since $deg_{G_1}^{u} = deg_{G}^{u} + 2$ and with respect to the above formulations, we have

$$HM(G_1) - HM(G_2) = 2\sum_{x\in N_G(u)} deg_{G}^{x} + 3(deg_{G}^{u})^2 + 13deg_{G}^{u} > 0.$$

[ii] $s \neq 2, t = 2$. In this case, we have

$$HM(G_1) = \sum_{xy\in E_1}\left(deg_{G_1}^{x} + deg_{G_1}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x}\right)^2 + \left(deg_{G_1}^{u} + deg_{G_1}^{u_2}\right)^2 + \left(deg_{G_1}^{u} + deg_{G_1}^{v_{s+1}}\right)^2 + 16(s-3) + 9.$$

Since $deg_{G_1}^{u_2} = 2$ and $deg_{G_1}^{v_{s+1}} = 1$, then

$$HM(G_1) = \sum_{xy\in E_1}\left(deg_{G}^{x} + deg_{G}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x}\right)^2 + \left(deg_{G_1}^{u} + 1\right)^2 + 16s - 39.$$

Moreover,

$$HM(G_2) = \sum_{xy\in E_1}\left(deg_{G_2}^{x} + deg_{G_2}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_2}^{u} + deg_{G}^{x}\right)^2 + \left(deg_{G_2}^{u} + deg_{G_2}^{u_2}\right)^2 + 16(s-2) + 9.$$

Since $deg_{G_2}^{u_2} = 2$, $deg_{G_2}^{u} = deg_{G_1}^{u} - 1$, then

$$HM(G_2) = \sum_{xy\in E_1}\left(deg_{G}^{x} + deg_{G}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x} - 1\right)^2 + \left(deg_{G_1}^{u} + 1\right)^2 + 16s - 23$$

Notice that, since $deg_{G_1}^{u} = deg_{G}^{u} + 2$ and with respect to $HM(G_1), HM(G_2)$, in this case, we have

$$HM(G_1) - HM(G_2) = 2\sum_{x\in N_G(u)} deg_{G}^{x} + 3(deg_{G}^{u})^2 + 11deg_{G}^{u} > 0$$

[iii] Finally, consider that $t = s = 2$, then we can obtain the following results in this case

$$HM(G_1) = \sum_{xy\in E_1}\left(deg_{G_1}^{x} + deg_{G_1}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x}\right)^2 + \left(deg_{G_1}^{u} + deg_{G_1}^{u_2}\right)^2 + \left(deg_{G_1}^{u} + deg_{G_1}^{v_{s+1}}\right)^2.$$

Since $deg_{G_1}^{u_2} = deg_{G_1}^{v_{s+1}} = 1$, we have

$$HM(G_1) = \sum_{xy\in E_1}\left(deg_{G}^{x} + deg_{G}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x}\right)^2 + 2\left(deg_{G_1}^{u} + 2\right)^2.$$

Moreover,

$$HM(G_2) = \sum_{xy\in E_1}\left(deg_{G_2}^{x} + deg_{G_2}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_2}^{u} + deg_{G}^{x}\right)^2 + \left(deg_{G_2}^{u} + deg_{G_2}^{u_2}\right)^2 + 9.$$

Since $deg_{G_2}^{u_2} = 2$, $deg_{G_2}^{u} = deg_{G_1}^{u} - 1$, then

$$HM(G_2) = \sum_{xy\in E_1}\left(deg_{G}^{x} + deg_{G}^{y}\right)^2 + \sum_{x\in N_G(u)}\left(deg_{G_1}^{u} + deg_{G}^{x} - 1\right)^2 + \left(deg_{G_1}^{u} + 1\right)^2 + 9.$$

Since $deg_{G_1}^{u} = deg_{G}^{u} + 2$ and with respect to the above formulations in this case, we have

$$HM(G_1) - HM(G_2) = 2\sum_{x\in N_G(u)} deg_G^x + 3(deg_G^u)^2 + 9deg_G^u > 0 . \blacksquare$$

Theorem 2. ([15]) If G is a connected graph, then

$$M_1(G) \geq \frac{4m^2}{n}\ ,\ \ M_2(G) \geq \frac{4m^3}{n^2}$$

Moreover, the equalities are attained if and only if the graph is regular.

3. The lower bound for Hyper-Zagreb index

In this section, we give a lower bound for Hyper-Zagreb index.

Example1. If G is a connected graph with n vertices, then the maximum of Hyper-Zagreb index is for $G = K_n$ by Lemma 1. Moreover, it is clear that P_n has a minimum of Hyper-Zagreb index among all connected graphs by using the Theorem 1, therefore

$16n - 30 = HM(P_n) \leq HM(G) \leq HM(K_n) = 2n(n-1)^3$.

Lemma 2. Let G be a connected graph, then

$(a). M_1(G) = \sum_{uv\in E(G)} deg_G^u\ ,\qquad (b). \sum_{uv\in E(G)} (deg_G^u)^2 = (deg_G^u)^3$

Proof. We can easily see that

$$\sum_{uv\in E(G)} deg_G^u = \sum_{u\in V(G)}\sum_{v\in N_G(u)} deg_G^u = \sum_{u\in V(G)} deg_G^u|N(u)| = \sum_{u\in V(G)} (deg_G^u)^2 = M_1(G).$$

Moreover, for part (b) we have

$$\sum_{uv\in E(G)} (deg_G^u)^2 = \sum_{v\in N_G(u)} (deg_G^u)^2 = (deg_G^u)^3\ .\ \blacksquare$$

Lemma 3. For the connected and simple graph G, the Hyper-Zagreb index of graph G is equal to

$$HM(G) = 2M_2(G) + \sum_{u\in V(G)} (deg_G^u)^3.$$

Proof. By definition of Hyper-Zagreb index graph G, we can have

$$\begin{aligned} HM(G) = &\sum_{e=uv\in E(G)} (deg_G^u + deg_G^v)^2 = \sum_{e=uv\in E(G)} (deg_G^u)^2 + 2deg_G^u.deg_G^v + (deg_G^v)^2 \\ &= \sum_{u\in V(G)} (deg_G^u)^3 + 2\sum_{e=uv\in E(G)} deg_G^u.deg_G^v = \sum_{u\in V(G)} (deg_G^u)^3 + 2M_2(G).\ \blacksquare \end{aligned}$$

Lemma 4. $HM(G)$ index is an even integer number.

Proof. By applying Lemma 3, it is enough to show that $\sum_{u\in V(G)}(deg_G^u)^3$ is an even number. We define sets A and B as follows

$$A = \{u|u \in V(G)\ , deg_G^u\ is\ an\ even\ number\}$$

$B = \{u|u \in V(G)\ , deg_G^v\ is\ an\ odd\ number\}$,

Since the sum of the degrees of the vertices of a graph is twice the number of edges, therefore $|A|$, $|B|$, $\sum_{u\in A}(deg_G^u)^3$ and $\sum_{u\in B}(deg_G^u)^3$ are even numbers, then $\sum_{u\in V(G)}(deg_G^u)^3 = \sum_{u\in A}(deg_G^u)^3 + \sum_{u\in B}(deg_G^u)^3$ is an even number, too. $\blacksquare$

Theorem 3. For Hyper-Zagreb index of a graph G, we have a lower bound as follows

$$HM(G) \geq \frac{4m}{n}M_1(G) + 2M_2(G)$$

Proof. If $a_1 \geq a_2 \geq \cdots \geq a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$ are real numbers, then

$$\sum_{i=1}^{n} a_i b_i \geq \frac{1}{n}\left(\sum_{i=1}^{n} a_i\right)\left(\sum_{i=1}^{n} b_i\right),$$

and the equality occurs when $a_1 = a_2 = \cdots = a_n$ or $b_1 = b_2 = \cdots = b_n$.

Let $(G) = \{v_1, v_2, \ldots, v_n\}$, $a_i = deg_G^{v_i}$ and $b_i = \left(deg_G^{v_i}\right)^2$ for $i = 1, 2, \ldots, n$, then

$$\sum_{v_i\in V(G)} \left(deg_G^{v_i}\right)^3 \geq \frac{1}{n}M_1(G)(2m).$$

By using Lemma 3, we have $HM(G) \geq \frac{4m}{n}M_1(G) + 2M_2(G)$. $\blacksquare$

Theorem 4. If G is a connected graph, then

$$HM(G) \geq \frac{4m}{n}\left(M_1(G) + \frac{2m^2}{n}\right).$$

Proof. The proof is completed by using the Theorems 2 and 3. ■

4. The upper bound for Hyper-Zagreb index

In this section, we determine two upper bounds for Hyper-Zagreb. We first prove an auxiliary lemma, then give two upper bounds.

Lemma 5. If G is a connected graph, then, for Zagreb indices, we have

$$M_2(G) \leq \Delta\, M_1(G)$$

Proof. Consider that Δ is the maximum degree of vertices of graph, then $deg_G^u . deg_G^v \leq deg_G^u . \Delta$, therefore, we have

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

Theorem 5. If $M_1(G)$ and $H(G)$ are first Zagreb and Hyper-Zagreb indices of graph G, respectively, then

$$HM(G) \leq 2\Delta\left(n\Delta^2 + M_1(G)\right)$$

Proof. For $u \in V(G)$, we have $deg_G^u \leq \Delta$, therefore

$$\sum_{u\in V(G)} (deg_G^u)^3 \leq \sum_{u\in V(G)} \Delta^3 = n\Delta^3$$

By using the Lemmas 2 and 5, we have

$$HM(G) \leq 2n\Delta^3 + 2\Delta M_1(G) = 2\Delta\left(n\Delta^2 + M_1(G)\right). \ ■$$

From the above results, we can get the following corollary.

Corollary 1. If $M_1(G)$ and $HM(G)$ are first Zagreb and Hyper-Zagreb indices of graph G, respectively, then

$$\frac{4m}{n} M_1(G) + 2M_2(G) \leq HM(G) \leq 2\Delta\left(n\Delta^2 + M_1(G)\right).$$

Theorem 6. Let G be a graph with n vertices, m edges, and first and second Zagreb indices $M_1(G)$ and $M_2(G)$, respectively. Then

$$\frac{4m}{n} M_1(G) + 2M_2(G) \leq HM(G) \leq 4M_2(G) + nM_1(G).$$

Proof. For a graph G with n vertices, m edges, and first and second Zagreb indices $M_1(G)$ and $M_2(G)$, we have

$$\begin{aligned}
HM(G) &= \sum_{u\in V(G)} (deg_G^u)^3 + 2M_2(G) \\
&= \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in N_G(u)} (deg_G^u)^2 + (deg_G^v)^2 + 2M_2(G) \\
&= \sum_{u\in V(G)} \sum_{v\in N_G(u)} deg_G^u . deg_G^v + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in N_G(u)} (deg_G^u - deg_G^v)^2 + 2M_2(G) \\
&= 4M_2(G) + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in N_G(u)} (deg_G^u - deg_G^v)^2 \\
&\leq 4M_2(G) + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (deg_G^u - deg_G^v)^2 \\
&= 4M_2(G) + \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (deg_G^u)^2 + (deg_G^v)^2 - \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} deg_G^u . deg_G^v \\
&= 4M_2(G) + nM_1(G) - 4m^2 \leq 4M_2(G) + nM_1(G). \ ■
\end{aligned}$$

4. Conclusions

In this paper, we studied the Hyper-Zagreb index which was introduced recently by Shirdel *et al.* [19]. Two upper bounds and a lower bound were given for the Hyper-Zagreb index. These upper and lower bounds for this index of graph G are associated with $n = |V(G)|$, $m = |E(G)|$, first and second Zagreb indices $M_1(G)$ and $M_1(G)$.

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