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Maximal hyper-Zagreb index of trees, unicyclic and bicyclic graphs with a given order and matching number

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Abstract

Let G be a simple connected graph. The hyper-Zagreb index is defined as $HM(G) = \sum_{uv\in E(G)}(d_G(u) + d_G(v))^2$. In this paper, the sharp upper bounds of the hyper-Zagreb index for trees, unicyclic and bicyclic graphs with a given order n and matching number α' are determined, and the graphs attaining these bounds are characterized.

Keywords: hyper-Zagreb index; tree; unicyclic graph; bicyclic graph; matching number.

2020 Mathematics Subject Classification: 05C07, 05C09, 05C92.

1. Introduction

In this paper, all graphs we considered are finite, undirected, and simple. Let G be an n-vertex graph with vertex set $V(G)$ and edge set $E(G)$. Let $|V|$ and $|E|$ be the number of vertices and edges of G, respectively. For a vertex $u \in V(G)$, the degree of u, denote by $d_u(G)$ (or shortly by d_u), is the number of vertices which are adjacent to u. Let $N_G(u)$ (or shortly $N(u)$) be the set of all neighbours of u in G. Call a vertex u a pendant vertex of G if $d_u = 1$ and denote by PV the set of pendent vertices of G, and call an edge uv a pendant edge of G, if $d_u = 1$ or $d_v = 1$. Denote by C_n and S_n the cycle and star on n vertices, respectively. Let $d_G(u, v)$ be the distance between vertices u and v in G. For $v \in V(G)$, let $G - v$ be a subgraph of G obtained from G by deleting a vertex v and its incident edges.

A connected graph G is called a unicyclic graph if it has a unique cycle. Bicyclic graphs are connected graphs with n vertices and $n + 1$ edges. For a unicyclic or bicyclic graph G, the forest obtained from G by deleting the edges of cycle(s) consists of several vertex-disjoint trees, each containing a vertex of the cycle(s), which is called the root of this tree in G.

A subset $M \subseteq E$ is called a matching in G if no two elements of M are adjacent. A matching M of G is said to be maximum, if for any other matching M' of G, $|M'| \leq |M|$. The matching number of G is the number of edges of a maximum matching in G. If M is a matching of G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be M-saturated, and if every vertex of G is M-saturated, then M is a perfect matching.

For a molecular graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined [8,9] as

$$M_1(G) = \sum_{uv\in V(G)} (d(u) + d(v)),$$

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

The first and second Zagreb index were first suggested by Gutman *et al.*, which absorbed attention of many scientists in different fields. See for instance [4,5,10,17] and the references therein.

In 2013, Shirdel *et al.* [20] introduced a new degree-based topological index named hyper-Zagreb index as

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

The hyper-Zagreb index is an important tool as it integrates the first and the second Zagreb indices. Gao *et al.* [6] found sharp bounds of the hyper-Zagreb index for acyclic, unicyclic, and bicyclic graphs. Liu *et al.* [15] obtained the maximum hyper-Zagreb index among cacti with perfect matchings. For more detail about this index, see [1,7,13,18].

Recently, the bounds of various indices for cacti, bicyclic graphs and other graphs with perfect matchings or with a given matching number have been studied. The lower bounds on augmented Zagreb index of trees and unicyclic graphs

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with perfect matchings are presented by Sun *et al.* [19]. Liu *et al.* [14, 16] obtained the minimum value of Szeged index and revised edge Szeged index among trees and unicyclic graphs with perfect matchings. Zhong *et al.* [23] determined minimum general sum-connectivity index of trees with given matching number. For other related results, see [3, 12].

In this paper, we determine the sharp upper bounds of the hyper-Zagreb index for trees, unicyclic and bicyclic graphs with a given order n and matching number α', and characterize the graphs attaining these bounds.

2. Main results

For the integers n and α' satisfying $n \geq 2\alpha'$, $\alpha' \geq 2$, let $\mathcal{T}(n,\alpha'),\mathcal{U}(n,\alpha')$ and $\mathcal{B}(n,\alpha')$, respectively, be the set of trees, unicyclic graphs and bicyclic graphs with n vertices and matching number α'. Firstly, we introduce some useful lemmas which will be used frequently.

Lemma 2.1. [11] *Let $G \in \mathcal{T}(2\alpha',\alpha')$, where $\alpha' \geq 2$, then G has at least two pendent vertices such that they are adjacent to vertices of degree 2, respectively.*

Lemma 2.2. [11] *Let $G \in \mathcal{T}(n,\alpha')$, where $n > 2\alpha'$, then there is an α'-matching M and a pendent vertex u such that u is not M-saturated.*

Lemma 2.3. [2] *Let $G \in \mathcal{U}(2\alpha',\alpha')$, where $\alpha' \geq 3$, and let T be a branch of G with root r. If $u \in V(T)$ is a pendent vertex which is furthest from the root r with $d(u,r) \geq 2$, then u is a adjacent to a vertex of degree two.*

Lemma 2.4. [21] *Let $G \in \mathcal{U}(n,\alpha')$, where $n > 2\alpha'$, and $G \neq C_n$, then there exists a maximum matching M and a pendant vertex u in G such that u is not M-saturated.*

Lemma 2.5. [22] *Let $G \in \mathcal{B}(2\alpha',\alpha')$, and $\alpha' \geq 3$, and T be a tree in G attached to a root r. If $v \in V(T)$ is a vertex furthest from the root r with $d_G(v,r) \geq 2$, then v is a pendent vertex and adjacent to a vertex u of degree two.*

Lemma 2.6. [22] *Let $G \in \mathcal{B}(n,\alpha')$, and $n > 2\alpha' \geq 6$, and G contains at least one pendent vertex, then there exist an α'-matching M and a pendent vertex u in G such that u is not M-saturated.*

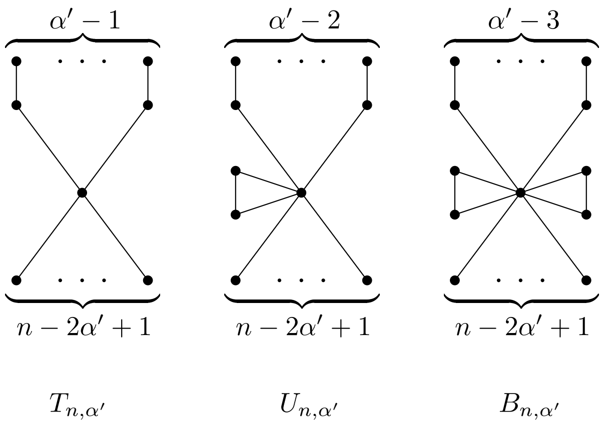

Figure 1: The graphs $T_{n,\alpha'}$, $U_{n,\alpha'}$ and $B_{n,\alpha'}$.

For $n \geq 2\alpha'$, $\alpha' \geq 2$, let $T_{n,\alpha'}$ (shown in Figure 1) be the tree obtained by attaching a pendent vertex to $\alpha' - 1$ noncentral vertices of the star $S_{n-\alpha'+1}$, and let $U_{n,\alpha'}$ (shown in Figure 1) be the unicyclic graph obtained by attaching $n - 2\alpha' + 1$ pendent vertices and $\alpha' - 2$ paths on two vertices to one vertex of a triangle, and let $B_{n,\alpha'}$ (shown in Figure 1) be the bicyclic graph of order n obtained by attaching $n - 2\alpha' + 1$ pendent vertices and $\alpha' - 3$ paths on two vertices to the common vertex of the two triangles. Obviously, $T_{n,\alpha'} \in \mathcal{T}(n,\alpha')$, $U_{n,\alpha'} \in \mathcal{U}(n,\alpha')$, and $B_{n,\alpha'} \in \mathcal{B}(n,\alpha')$. By the definition of the hyper-Zagreb index, we have that

$$HM(T_{n,\alpha'}) = (n - 2\alpha' + 1)(n - \alpha' + 1)^2 + (\alpha' - 1)(n - \alpha' + 2)^2 + 9\alpha' - 9.$$

$$HM(U_{n,\alpha'}) = \alpha'(n - \alpha' + 3)^2 + (n - 2\alpha' + 1)(n - \alpha' + 2)^2 + 9\alpha' - 2.$$

$$HM(B_{n,\alpha'}) = (n - 2\alpha' + 1)(n - \alpha' + 3)^2 + (\alpha' + 1)(n - \alpha' + 4)^2 + 9\alpha' + 5.$$

Lemma 2.7. [15] *If $G \in \mathcal{T}(2\alpha', \alpha')$, where $\alpha' \geq 2$, then*

$$HM(G) \leq (\alpha')^3 + 4(\alpha')^2 + 11\alpha' - 12,$$

with equality if and only if $G \cong T_{2\alpha',\alpha'}$.

In the following, we give sharp upper bound for the hyper-Zagreb index of tree with a given matching number.

Theorem 2.1. *If $G \in \mathcal{T}(n, \alpha')$, where $n \geq 2\alpha'$, $\alpha' \geq 2$, then*

$$HM(G) \leq (n - 2\alpha' + 1)(n - \alpha' + 1)^2 + (\alpha' - 1)(n - \alpha' + 2)^2 + 9\alpha' - 9,$$

with equality if and only if $G \cong T_{n,\alpha'}$ (shown in Figure 1).

Proof. We prove this result by using induction on n. When $n = 2\alpha'$, by Lemma 2.7, the theorem holds. Next, we consider $n > 2\alpha'$, and assume that the result holds for the graphs in $\mathcal{T}_{n-1,\alpha'}$. By Lemma 2.2, there exist a maximum matching M and a pendent vertex u such that u is not M-saturated. Let w be the unique neighbor of u and $N(w) \bigcap PV = \{u, u_1, u_2, \dots, u_{t-1}\}$, where PV is the set of all pendent vertices in G. Let $d_w = d$ and $N(w) \setminus PV = \{x_1, x_2, \dots, x_{d-t}\}$.

As M contains one edge incident with w and there are $n - \alpha' - 1$ edges outside M, so we have that $d - 1 \leq n - \alpha' - 1$, i.e., $d \leq n - \alpha'$. We known that $\sum_{v \in V(G)} d_v = 2|E|$, so we have

$$\sum_{i=1}^{d-t} d_{x_i} + d + t + (n - d - 1) \leq 2|E| = 2n - 2,$$

so

$$\sum_{i=1}^{d-t} d_{x_i} \leq n - t - 1.$$

Let $G^* = G - u$, as u is not M-saturated, then $G^* \in \mathcal{T}_{n-1,\alpha'}$. By the inductive assumption, $HM(G^*) \leq HM(T_{n-1,\alpha'})$.

$$\begin{aligned} HM(G) &= HM(G^*) + (t-1)[(d+1)^2 - d^2] + (d+1)^2 + \sum_{i=1}^{d-t}[(d + d_{x_i})^2 - (d + d_{x_i} - 1)^2] \\ &\leq HM(T_{n-1,\alpha'}) + 3d^2 - d + 2n - 2 \\ &= HM(T_{n,\alpha'}) + 3[d^2 - (n - \alpha')^2] + [(n - \alpha') - d] \\ &\leq HM(T_{n,\alpha'}). \end{aligned}$$

The equality $HM(G) = HM(T_{n,\alpha'})$ holds if and only if equalities hold throughout the above inequalities, i.e., $HM(G^*) = HM(T_{n-1,\alpha'})$, $d = n - \alpha'$, and $V(G) \setminus \{N(w) \bigcup \{w\}\}$ are pendent vertices. So we have that $HM(G) \leq HM(T_{n,\alpha'})$ with equality if and only if $G \cong T_{n,\alpha'}$. The proof is completed. □

Lemma 2.8. [6] *If G is a unicyclic graph with n vertices, then*

$$HM(C_n) \leq HM(G),$$

with equality if and only if $G \cong C_n$.

Lemma 2.9. [15] *If $G \in \mathcal{U}(2\alpha', \alpha')$, where $\alpha' \geq 2$, then*

$$HM(G) \leq (\alpha')^3 + 7(\alpha')^2 + 22\alpha' + 2,$$

with equality if and only if $G \cong U_{2\alpha',\alpha'}$.

Next we give sharp upper bound for the hyper-Zagreb index of unicyclic graph with a given matching number.

Theorem 2.2. *If $G \in \mathcal{U}(n, \alpha')$, where $n \geq 2\alpha'$, $\alpha' \geq 2$, then*

$$HM(G) \leq \alpha'(n - \alpha' + 3)^2 + (n - 2\alpha' + 1)(n - \alpha' + 2)^2 + 9\alpha' - 2,$$

with equality if and only if $G \cong U_{n,\alpha'}$ (shown in Figure 1).

Proof. Again we use induction on n. When $n = 2\alpha'$, by Lemma 2.9, the theorem holds. Next, we consider $n > 2\alpha'$, and assume that the result holds for the graphs in $\mathcal{U}(n-1, \alpha')$.

Case 1 $G = C_n$.
By Lemma 2.8, one knows that C_n is the graph with minimum hyper-Zagreb index.

Case 2 $G \neq C_n$.
By Lemma 2.4, there exist a maximum matching M and a pendent vertex u such that u is not M-saturated. Let w be the unique neighbor of u and $N(w) \bigcap PV = \{u, u_1, u_2, \ldots, u_{t-1}\}$, where PV is the set of all pendent vertices in G. Let $d_w = d$ and $N(w) \setminus PV = \{x_1, x_2, \ldots, x_{d-t}\}$.

As M contains one edge incident with w and there are $n - \alpha'$ edges outside M, so we have that $d - 1 \leq n - \alpha'$, i.e., $d \leq n - \alpha' + 1$.

We known that $\sum_{v \in V(G)} d_v = 2|E|$, so we have

$$\sum_{i=1}^{d-t} d_{x_i} + d + t + (n - d - 1) \leq 2|E| = 2n,$$

so

$$\sum_{i=1}^{d-t} d_{x_i} \leq n - t + 1.$$

Let $G^* = G - u$, as u is not M-saturated, then $G^* \in \mathcal{U}(n-1, \alpha')$. By the inductive assumption, $HM(G^*) \leq HM(U_{n-1,\alpha'})$.

$$\begin{aligned} HM(G) &= HM(G^*) + (t-1)[(d+1)^2 - d^2] + (d+1)^2 \\ &\quad + \sum_{i=1}^{d-t}[(d + d_{x_i})^2 - (d + d_{x_i} - 1)^2] \\ &\leq HM(U_{n-1,\alpha'}) + 3d^2 - d + 2n + 2 \\ &= HM(U_{n,\alpha'}) + 3[d^2 - (n - \alpha' + 1)^2] + [(n - \alpha' + 1) - d] \\ &\leq HM(U_{n,\alpha'}). \end{aligned}$$

The equality $HM(G) = HM(U_{n,\alpha'})$ holds if and only if equalities hold throughout the above inequalities, i.e., $HM(G^*) = HM(U_{n-1,\alpha'})$, $d = n - \alpha' + 1$, and $V(G) \setminus \{N(w) \bigcup \{w\}\}$ are pendent vertices. So we have that $HM(G) \leq HM(U_{n,\alpha'})$ with equality if and only if $G \cong U_{n,\alpha'}$. The proof is completed. □

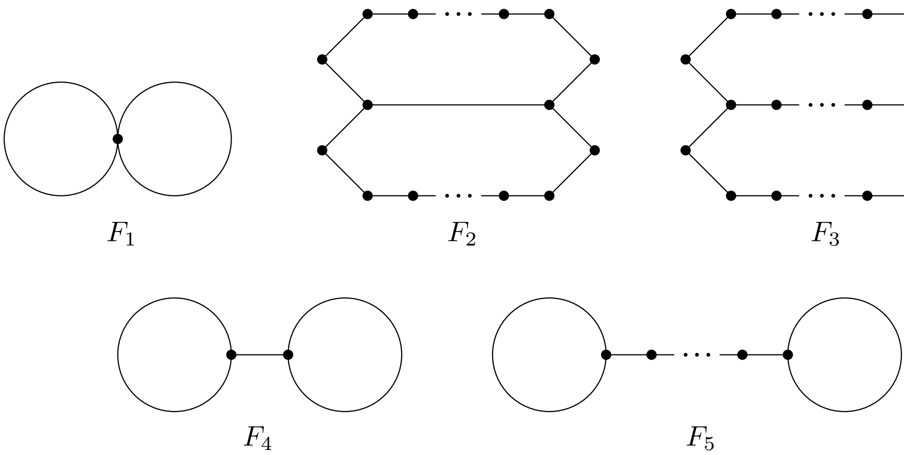

Figure 2: The graphs of the class $\{F_i \ : \ 1 \leq i \leq 5\}$.

Theorem 2.3. *If* $G \in \mathcal{B}(2\alpha', \alpha')$, $\alpha' \geq 3$, *then*

$$HM(G) \leq (\alpha' + 3)^2 + (\alpha' + 1)(\alpha' + 4)^2 + 9\alpha' + 5,$$

with equality if and only if $G \cong B_{2\alpha', \alpha'}$.

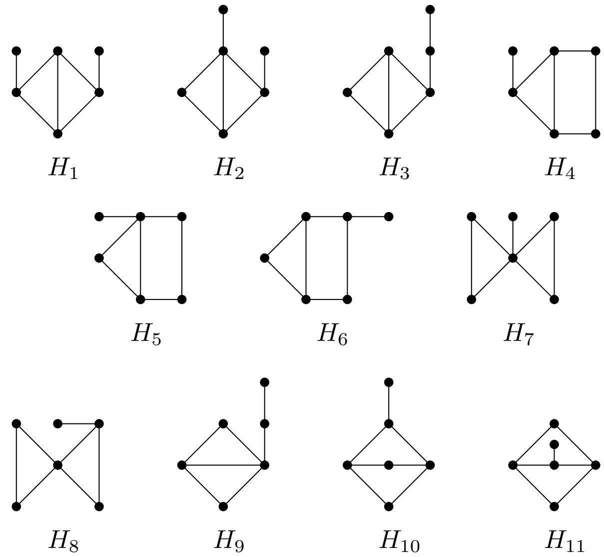

Figure 3: The graphs of the class $\{H_i \ : \ 1 \leq i \leq 11\}$.

Proof. Let $f(2\alpha', \alpha') = (\alpha'+3)^2 + (\alpha'+1)(\alpha'+4)^2 + 9\alpha' + 5$. If $PV(G) = \emptyset$, then $G \in \{F_i \ : \ 1 \leq i \leq 5\}$, (see Figure 2), and $n = 2\alpha'$. By calculating directly, we have that

$$HM(F_1) = 32\alpha' + 80, HM(F_2) = 32\alpha' + 56, HM(F_3) = 32\alpha' + 54, HM(F_4) = 32\alpha' + 56, HM(F_5) = 32\alpha' + 54.$$

Obviously, we have that $HM(F_i) < HM(B_{2\alpha',\alpha'})$ $(\alpha' \geq 3)$, for $1 \leq i \leq 5$.

Next, we assume that $PV(G) \neq \emptyset$.

We prove the result by induction on α'. When $\alpha' = 3$, all graphs of the class $\mathcal{B}(6,3) = \{H_i \ : \ 1 \leq i \leq 11\}$ are shown in Figure 3. Though calculating directly, $HM(H_1) = 212$, $HM(H_2) = 236$, $HM(H_3) = 192$, $HM(H_4) = 190$, $HM(H_5) = 212$, $HM(H_6) = 188$, $HM(H_7) = 264$, $HM(H_8) = 214$, $HM(H_9) = 226$, $HM(H_{10}) = HM(H_{11}) = 188$. We known that $H(G) \leq f(6,3)$ with equality if and only if $G \cong B_{6,3}$.

Next, we assume that $\alpha' \geq 4$, and the conclusion is true for $\mathcal{B}(2k,k)$ $(k < \alpha')$. Let T_i be a tree in G which attached at the root r_i $(i = 1, 2, \dots)$. Let $v_i \in PV(T_i)$ be farthest from the root r_i. We consider the following two cases to prove our results.

Case 1 $d_{T_i}(r_i, v_i) = 1$ for all $T_i \in G$.

Subcase 1.1 $d_v \neq 2$ for all vertex $v \in V(G)$.

As $d_v \neq 2$ for all vertex $v \in V(G)$, one has $G \in \{B_i \ : \ 1 \leq i \leq 7\}$, bicyclic graphs B_i $(1 \leq i \leq 7)$ are shown in Figure 4. By calculating directly, we have that $HM(B_1) = 52\alpha' + 168$, $HM(B_2) = 52\alpha' + 56$, $HM(B_3) = 52\alpha' + 134$, $HM(B_4) = 52\alpha' + 132$, $HM(B_5) = 52\alpha' + 56$, $HM(B_6) = 52\alpha' + 134$, $HM(B_7) = 52\alpha' + 132$. We have that $HM(B_i) < HM(B_{2\alpha',\alpha'})$ $(\alpha' \geq 4)$, for $1 \leq i \leq 7$.

Subcase 1.2 $d_v = 2$ for several $v \in V(G)$.

Subcase 1.2.1 There is no vertex of degree two which lie in any cycle of G.

As $d_{T_i}(r_i, v_i) = 1$ for all $T_i \in G$, and there is no vertex of degree two which lie in any cycle of G. Note that there exist $u_2u_3 \in E(G)$ which belongs to one of the cycles in G such that $d_{u_2} = d_{u_3} = 3$. Let $N(u_2) = \{u_1, u_3, v_2\}$, $N(u_3) = \{u_2, u_4, v_3\}$. Without loss of generality, we suppose that $d_{v_2} = d_{v_3} = 1$, $3 \leq d_{u_1} \leq 4$, and $3 \leq d_{u_4} \leq 4$. Let $G^* = G - u_2u_3$, then $G^* \in \mathcal{U}(2\alpha', \alpha')(\alpha' \geq 6)$. By the inductive assumption, we have that

$$\begin{aligned} HM(G) &= HM(G^*) + ((d_{u_1}+3)^2 - (d_{u_1}+2)^2) + ((d_{u_4}+3)^2 - (d_{u_4}+2)^2) \\ &\leq HM(U_{2\alpha',\alpha'}) + 2d_{u_1} + 2d_{u_4} + 60 \\ &= HM(B_{2\alpha',\alpha'}) - [3(\alpha')^2 + 17\alpha' + 19] + [2d_{u_1} + 2d_{u_4} + 60] \\ &< HM(B_{2\alpha',\alpha'}). \end{aligned}$$

Subcase 1.2.2 There exists a vertex of degree two which lies on one of the cycles of G.

Suppose that the vertex u_2 with degree 2 lie in one of cycles of G, and $N(u_2) = \{u_1, u_3\}$. As $G \in \mathcal{B}(2\alpha', \alpha')$, there exists an edge between u_1u_2 and u_2u_3 that are not belong to an α'-matching. Without loss of generality, we suppose that edge u_2u_3 is not belong to the α'-matching. Let $d_{u_3} = d$, and $N(u_3) \setminus \{u_2\} = \{x_1, x_2, \dots, x_{d-1}\}$. Obviously, one has $2 \leq d \leq 5$, $2 \leq d_{u_1} \leq 5$.

Let $G^* = G - u_2u_3$, then $G^* \in \mathcal{U}_{2\alpha',\alpha'}$. We know that $\sum_{v\in V(G)} d_v = 2|E|$, so we have

$$\sum_{i=1}^{d-1} d_{x_i} + d + d_{u_1} + 2 + (2\alpha' - d - 2) \le 2|E| = 2(2\alpha' + 1),$$

so $\sum_{i=t}^{d-1} d_{x_i} \le 2\alpha' - d_{u_1} + 2$. By the inductive assumption, $HM(G^*) \le HM(U_{2\alpha',\alpha'})$, and hence we have that

$$\begin{aligned} HM(G) &= HM(G^*) + \sum_{i=1}^{d-1}[(d+d_{x_i})^2 - (d+d_{x_i}-1)^2] + (d_{u_1}+2)^2 - (d_{u_1}+1)^2 + (d+2)^2 \\ &\le HM(U_{2\alpha',\alpha'}) + 3d^2 + d + 12 \\ &= HM(B_{2\alpha',\alpha'}) - (3(\alpha')^2 + 17\alpha' + 19) + 3d^2 + d + 12 \\ &< HM(B_{2\alpha',\alpha'}). \end{aligned}$$

where the last inequality holds for $\alpha' \ge 4$ and $2 \le d \le 5$.

Case 2 $d_{T_i}(r_i, v_i) \ge 2$ for several $T_i \in G$.
Since $v_i \in PV(G)$, let $N(v_i) = u$. By Lemma 2.5, one has $d_u = 2$. Let $N(u) = \{v_i, w\}$, $N(w) \bigcap PV = \{x_1, x_2, \ldots, x_t\}$, $N(w) \setminus PV = \{x_{t+1}, x_{t+2} \ldots, x_{d-1}, x_d = u\}$. As M contains exactly one edge incident with w and there α' edges of G outside M, we have that $d-1 \le \alpha' - 1$, i.e., $d \le \alpha' + 2$. $d_{x_i} \ge 2$, $i = t+1, \ldots, d-1$.

Let $G^* = G - v_i - u$, then $G^* \in \mathcal{B}(2(\alpha'-1), \alpha'-1)$. By the inductive assumption, $HM(G^*) \le f(2(\alpha'-1), \alpha'-1)$. We know that $\sum_{v\in V(G)} d_v = 2|E|$, so we have $\sum_{i=t+1}^{d-1} d_{x_i} + d + t + 3 + (2\alpha' - d - 2) \le 2|E| = 2(2\alpha'+1)$, so $\sum_{i=t+1}^{d-1} d_{x_i} \le 2\alpha' - t + 1$.

$$\begin{aligned} HM(G) &= HM(G^*) + \sum_{i=t+1}^{d-1}[(d+d_{x_i})^2 - (d+d_{x_i}-1)^2] + t[(d+1)^2 - d^2] + (d+2)^2 + 9 \\ &\le f(2\alpha',\alpha') + [f(2(\alpha'-1),\alpha'-1) - f(2\alpha',\alpha')] + 3d^2 + d + 4\alpha' + 16 \\ &= f(2\alpha',\alpha') + 3(d^2 - (\alpha'+2)^2) + (d - (\alpha'+2)) \\ &\le f(2\alpha',\alpha'). \end{aligned}$$

The equality $HM(G) = f(2\alpha',\alpha')$ holds if and only if equalities hold throughout the above inequalities, i.e., $HM(G^*) = f(2(\alpha'-1),\alpha'-1)$, $d = \alpha'+2$, and $V(G) \setminus \{N(w) \bigcup \{w\} \bigcup \{v_i\}\}$ are pendent vertices. So we have that $HM(G) \le f(2\alpha',\alpha')$ with equality if and only if $G \cong B_{2\alpha',\alpha'}$ (shown in Figure 1). The proof is completed. □

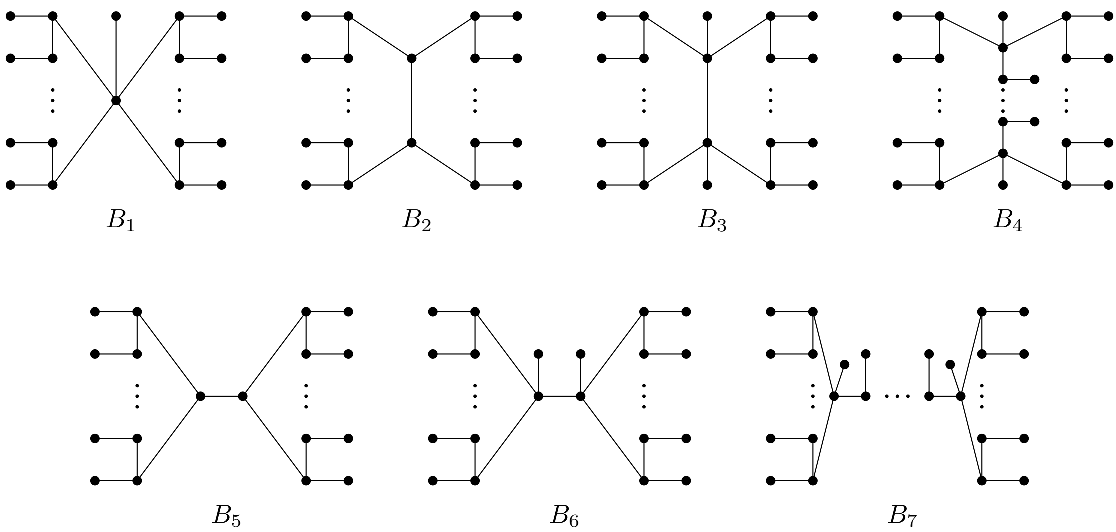

Figure 4: The graphs of the class $\{B_i \ : \ 1 \le i \le 7\}$.

Next we give sharp upper bound for the hyper-Zagreb index of bicyclic graph with a given matching number.

Theorem 2.4. *If $G \in \mathcal{B}(n,\alpha')$, where $n \ge 2\alpha'$, $\alpha' \ge 3$, then*

$$HM(G) \le (n - 2\alpha' + 1)(n - \alpha' + 3)^2 + (\alpha'+1)(n - \alpha' + 4)^2 + 9\alpha' + 5,$$

with equality if and only if $G \cong B_{n,\alpha'}$.

Proof. Let $g(n,\alpha') = (n-2\alpha'+1)(n-\alpha'+3)^2 + (\alpha'+1)(n-\alpha'+4)^2 + 9\alpha' + 5$. We prove the result by induction on n. If $n = 2\alpha'$, the result follows from Theorem 2.3. Next, we assume that $n > 2\alpha'$ and the result holds for all bicyclic graphs on fewer than n vertices. Let $G \in \mathcal{B}(n,\alpha')$.

Case 1 $PV(G) = \emptyset$.
As there is no pendent vertex in G which has an α'-matching, then $G \in \{F_i \ : \ 1 \le i \le 5\}$ (see Figure 3), and $n = 2\alpha' + 1$. By direct calculations, one has $HM(F_1) = 32\alpha' + 112$, $HM(F_2) = 32\alpha' + 88$, $HM(F_3) = 32\alpha' + 86$, $HM(F_4) = 32\alpha' + 88$, $HM(F_5) = 32\alpha' + 86$. $HM(F_i) < g(2\alpha'+1,\alpha')$, for $1 \le i \le 5$.

Case 2 $PV(G) \neq \emptyset$.
By Lemma 2.6, G has an α'-matching M and there exist $v \in PV(G)$ such that v is M-unsaturated. Let $N(v) = \{u\}$, and $d_u = d$. Let $N(u) \bigcap PV = \{v_1, v_2, \ldots, v_{t-1}, v_t = v\}$, and $N(u) \setminus PV = \{x_t, x_{t+1}, \ldots, x_{d-1}\}$. As M contains exactly one edge incident with v and there $n+1-\alpha'$ edges of G outside M, we have that $d-1 \le n+1-\alpha'$, i.e., $d \le n-\alpha'+2$.

Let $G^* = G - v$, then $G^* \in \mathcal{B}(n-1,\alpha')$. By the inductive assumption, $HM(G^*) \le g(n-1,\alpha')$. We know that $\sum_{v\in V(G)} d_v = 2|E|$, so we have $\sum_{i=t}^{d-1} d_{x_i} + d + t + (n-d-1) \le 2|E| = 2(n+1)$, so $\sum_{i=t}^{d-1} d_{x_i} \le n - t + 3$.

$$\begin{aligned}
HM(G) &= HM(G^*) + \sum_{i=t}^{d-1}[(d+d_{x_i})^2 - (d+d_{x_i}-1)^2] + (d+1)^2 + (t-1)[(d+1)^2 - d^2] \\
&\le g(n,\alpha') + [g(n-1,\alpha') - g(n,\alpha')] + 3d^2 - d + 2n + 6 \\
&= g(n,\alpha') + 3(d^2 - (n-\alpha'+2)^2) + ((n-\alpha'+2) - d) \\
&\le g(n,\alpha').
\end{aligned}$$

The equality $HM(G) = g(n,\alpha')$ holds if and only if equalities hold throughout the above inequalities, i.e., $HM(G^*) = g(n-1,\alpha')$, $d = n-\alpha'+2$, and $V(G) \setminus \{N(u) \bigcup \{u\}\}$ are pendent vertices. So we have that $HM(G) \le g(n,\alpha')$ with equality if and only if $G \cong B_{n,\alpha'}$. The proof is completed. □

3. Conclusion

In this paper, we determine the sharp upper bounds of the hyper-Zagreb index for trees, unicyclic and bicyclic graphs with a given order n and matching number α', and characterize the graphs attaining these bounds. Motivated by [23], it is also interesting to obtain the bounds of general sum-connectivity index for trees, unicyclic and bicyclic graphs with a given order n and matching number α'. We intend to consider this problem in the near future.

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