Maximum first Zagreb index of orientations of unicyclic graphs with given matching number

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Abstract

Let D = (V, A) be a digraphs without isolated vertices. The first Zagreb index of a digraph D is defined as a summation over all arcs, $M_1(D) = \frac{1}{2} \sum_{uv \in A} (d_u^+ + d_v^-)$, where d_u^+ (resp. d_u^-) denotes the out-degree (resp. in-degree) of the vertex u. In this paper, we give the maximal values and maximal digraphs of first Zagreb index over the set of all orientations of unicyclic graphs with n vertices and matching number $m \ (2 \le m \le \lfloor \frac{n}{2} \rfloor)$.

Keywords: first Zagreb index; orientations of unicyclic graphs; matching number.

1 Introduction

The first Zagreb index was first appeared in [1, 2], and it is an important molecular descriptor which is related with many chemical properties. The first Zagreb index have been used in the study of molecular complexity, chirality, ZE-isomerism and heterosystems whilst the Zagreb indices played a potential role in applicability for deriving multilinear regression models. Zagreb indices are also used by researchers in the studies of QSPR and QSAR [11]. During the past decades, results closely correlated with the Zagreb indices have published in [3, 4, 5, 6, 7, 8, 9].

We denote by G = (V, E) a simple connected graph, where V(G) is the vertex set of G and E(G) is the edge set of G. The first Zagreb index of G is defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$$

where $d_G(v)$ (d_v for short) is the degree of vertex v in G.

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For any $v \in V(G)$, let $N_G(v) = \{u | uv \in E(G)\}$ be the neighbors of v, and $d_G(v) \doteq |N_G(v)|$ the degree of v in G. For $E' \subseteq E(G)$, G - E' denotes the subgraph of G obtained by deleting the edges of E'. Let $W \subseteq V(G)$, we denote by G - W the subgraph of Gobtained by deleting the vertices of W and the edges incident with them. A matching Mof the graph G is a subset of E(G) such that no two edges in M share a common vertex. A matching M of G is maximum, if $|M_1| \leq |M|$ for any other matching M_1 of G. The matching number of G is the number of edges of a maximum matching in G. If M is a matching of a graph G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be M-saturated, and if any $v \in V(G)$ is M-saturated, then M is a perfect matching.

A digraph D = (V, A) is an ordered pair (V, A) consisting of a non-empty finite set Vof vertices and a finite set A of ordered pairs of distinct vertices called arcs (in particular, D has no loops). Let $uv \in A$, we denote by uv an arc from vertex u to vertex v. The vertex u is the tail of uv, and the vertex v is its head. d_u^+ (resp. d_u^-) denotes the out-degree (resp. in-degree) of a vertex u which is the number of arcs with tail u (resp. with head u). If $u \in V$ and $d_u^+ = d_u^- = 0$, then u is called an isolated vertex. D_n denotes the set of all digraphs with n non-isolated vertices. The first Zagreb index of a digraph D defined as

$$M_1(D) = \frac{1}{2} \sum_{uv \in A} (d_u^+ + d_v^-)$$

where $d_u^+(\text{resp. } d_u^-)$ denotes the out-degree(resp.in-degree) of the vertex u. If $u \in V(D)$ and $d_u^+ = 0$ (resp. $d_u^- = 0$), then u is called a sink vertex (resp. source vertex). An oriented graph D is obtained from a graph G by replacing each edge uv of G by an arc uv or vu, but not both. In this case D is also called an orientation of G. Let $\mathcal{O}(G)$ be the set of all orientations of G. $D \in \mathcal{O}(G)$, if $d_u^+ = 0$ or $d_u^- = 0$ for any $u \in V(D)$, then Dis called a sink-source orientation of G.

In order to better study of vertex-degree-based topological indices. Recently, J. Monsalve and J. Rada [12] extended the concept of vertex-degree based topological indices of graphs to oriented graphs. the authors determined the extremal values of the Randić index over $\mathcal{OT}(n)$, the set of all oriented trees with n vertices. Also, the authors given the extremal values of the Randić index over $\mathcal{O}(P_n), \mathcal{O}(C_n)$ and $\mathcal{O}(H_d)$, where P_n is the path with n, P_n is the cycle with n vertices and H_d is the hypercube of dimension d, respectively. J. Monsalve and J. Rada [14] found extremal values of symmetric VDB topological indices over $\mathcal{OT}(n)$ and $\mathcal{O}(G)$, respectively. But the maximum value of \mathcal{AZ} over $\mathcal{OT}(n)$ is still an open problem.

In this paper, we present the maximal first Zagreb index for orientations of unicyclic graphs with n vertices and matching number m $(2 \le m \le \lfloor \frac{n}{2} \rfloor)$, and we state the results as follows:

Let n and m be integers and $2 \le m \le \lfloor \frac{n}{2} \rfloor$, U(n,m) the class of unicyclic graphs on n

vertices with matching number m, and $U_{n,m}$ the graph formed by attaching n - 2m + 1pendent vertices and m - 2 paths of length 2 to a (common) vertex of a triangle. Let $U_{n,m}^{(1)}, U_{n,m}^{(2)}, U_{n,m}^{(3)}, U_{n,m}^{(4)}$ be four orientations of $U_{n,m}$ (see Figure 1). Obviously, $U_{n,m} \in U(n,m)$. Let C_n be the the cycle with n vertices. $U_{4,2}^* = \{U_{4,2}^{(1)}, U_{4,2}^{(2)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}, U_{4,2}^{(5)}, U_{4,2}^{(6)}\},$ where $U_{4,2}^{(5)}$ and $U_{4,2}^{(6)}$ are the sink-sourse orientations of C_4 . $U_{6,3}^* = \{U_{6,3}^{(1)}, U_{6,3}^{(2)}, U_{6,3}^{(3)}, U_{6,3}^{(4)}, U_{6,3}^{(5)}, U_{6,3}^{(6)}, U_{6,3}^{(6)}\},$ where $U_{6,3}^{(5)}$ and $U_{6,3}^{(6)}$ are the sink-sourse orientations of the graph formed by attaching two pendant vertices to two adjacent vertices of C_4 . $U_{n,m}^* = \{U_{n,m}^{(1)}, U_{n,m}^{(2)}, U_{n,m}^{(3)}, U_{n,m}^{(4)}\},$ where $(n,m) \neq (4,2), (6,3)$.



Figure 1: Four orientations of $U_{n,m}: U_{n,m}^{(1)}, U_{n,m}^{(2)}, U_{n,m}^{(3)}, U_{n,m}^{(4)}$

Theorem 1. Let $G \in U(n,m)$ with $2 \le m \le \lfloor \frac{n}{2} \rfloor$, $D \in \mathcal{O}(G)$. Then

$$M_1(D) \le \frac{1}{2} \left[n^2 + (-2m+3)n + m^2 + m - 2 \right]$$

with equality if and only if $D \in U_{n,m}^*$.

Specially, if n = 2m, we have

Theorem 2. Let $G \in U(2m, m)$ with $m \ge 2$, $D \in \mathcal{O}(G)$. Then

$$M_1(D) \le \frac{1}{2}[m^2 + 7m - 2]$$

with equality if and only if $G \in U^*_{2m,m}$.

Hence, we solve the problem on the maximum values of the first Zagreb index for orientations of unicyclic graphs with n vertices and matching number $m \ (2 \le m \le \lfloor \frac{n}{2} \rfloor)$.

2 Some useful lemmas

In this section, we give three useful lemmas.

Lemma 3. [13] Let G be a graph. Then G is a bipartite graph if and only if G has a sink-source orientation. Moreover, If G is a connected bipartite graph, then there exist exactly two sink- source orientations of G.

Now, we can show a important result.

Lemma 4. Let G be a graph, $D \in \mathcal{O}(G)$. Then

$$M_1(D) \le \frac{M_1(G)}{2}$$

equality occurs if and only if D is a sink-source orientation of G.

Proof. Let G = (V, E) and D = (V, A). For each $u \in V$, $d_u = d_u^+ + d_u^-$. So $d_u \ge d_u^+$ and $d_v \ge d_v^-$, where $u, v \in V$. Then $d_u^+ + d_v^- \le d_u + d_v$. Hence

$$M_1(D) = \frac{1}{2} \sum_{uv \in A} (d_u^+ + d_v^-) \le \frac{1}{2} \sum_{uv \in E(G)} (d_u + d_v) = \frac{M_1(G)}{2}.$$

If D is a sink-source orientation of G, then for each $u \in V$, one has either $d_u^+ = 0$ or $d_u^- = 0$. Moreover, if $uv \in A$, then $d_u^+ \neq 0$ and $d_u^- = 0$, so $d_u = d_u^+$. It is Similar to d_v . Hence

$$M_1(D) = \frac{1}{2} \sum_{uv \in A} (d_u^+ + d_v^-) = \frac{1}{2} \sum_{uv \in E(G)} (d_u + d_v) = \frac{M_1(G)}{2}$$

Conversely, $d_u \ge d_u^+$ and $d_v \ge d_v^-$, then $d_u + d_v \ge d_u^+ + d_v^-$ with equality if and only if $d_u = d_u^+$ and $d_v = d_v^-$, so $M_1(D) = \frac{M_1(G)}{2}$ if and only if $d_u = d_u^+$ and $d_v = d_v^-$, where all $uv \in A$. This clearly implies that either $d_w^+ = 0$ or $d_w^- = 0$ for any $w \in V$.

Lemma 5. Let G be the graph with n non-islated vertices and $D \in \mathcal{O}(G)$. Then

$$M_1(D) = \frac{1}{2} \sum_{u \in V(D)} \left[(d_u^+)^2 + (d_u^-)^2 \right]$$

Proof. As the fact that $M_1(D) = \frac{1}{2} \sum_{uv \in A} [(d_u^+) + (d_v^-)]$ and d_u^+ (resp. d_u^-) occur d_u^+ (resp. d_u^-) times in the sum, for each $u \in V(D)$.

So, $M_1(D) = \frac{1}{2} \sum_{u \in V(D)} \left[(d_u^+)^2 + (d_u^-)^2 \right].$

3 Proof of Theorem 2

In this section, we first give a proof of Theorem 2, then we will prove Theorem 1 in next section by using Theorem 2.

We first determine the maximum values of the first Zagreb index for orientations of trees with 2m vertices and matching number $m \ (m \ge 1)$.

Let n and m be integers and $1 \le m \le \lfloor \frac{n}{2} \rfloor$. T(n,m) denotes the class of trees on n vertices with matching number m. We denote by $T_{n,m}$ a tree formed by attaching a pendent vertex to each of m-1 pendent vertices of the graph $K_{1,n-m}$, where a pendent vertex is a vertex of degree one (see Figure 2). Obviously, $T_{n,1} = K_{1,n-1}$ and $T_{n,m} \in T(n,m)$. Let T be a tree with $u, v \in V(T)$. We denote by $P_T(u,v)$ the unique path from u to v in T. Firstly, we give a lemma which is related to $P_T(u,v)$.



Figure 2: The graph $T_{n,m}$.

Lemma 6. [15] Let T be a tree with at least four vertices and a perfect matching M. If $P_T(u, v)$ as a diametrical path in T, then the unique neighbor of u has degree two.

We first consider trees with a perfect matching.

Lemma 7. Let $T \in T(2m, m)$ with $m \ge 1$. Then

$$M_1(T) \le m^2 + 5m - 4$$

with equality if and only $T \cong T_{2m,m}$.

Proof. We will prove by induction on m.

Obviously, $T = T_{2,1}$ for m = 1, and $T = T_{4,2}$ for m = 2. So the result holds for m = 1, 2.

If $m \geq 3$. Suppose that the result holds for trees in T(2(m-1), (m-1)). Let $T \in T(2m, m)$ and M a perfect matching of T. Note that the diameter of T is at least four. We can denote by $P_T(u, v) = uxyz \cdots$ a diametrical path in T. Then $z \neq v$. Let $N_T(y) = \{x_1, x_2, \dots, x_{s+1}\}$ with $x_1 = x$ and $x_{s+1} = z$.

Suppose that $yz \in M$. By Lemma 6, $d_{x_i} = 2$ and $d_{u_i} = 1$, where u_i is the neighbor of x_i different from y for $1 \le i \le s$, and $u_1 = u$. So $2(2m-1) \ge \sum_{i=1}^{s} (d_{x_i} + d_{u_i}) + d_y + d_z + d_v \ge 3s + (s+1) + 2 + 1 > 4s + 2$, hence s < m - 1. Suppose that $yz \notin M$. Then M contains zw for some neighbor w of z different from y, and M contains one of yx_i for $2 \le i \le s$, say yx_s . Since $P_T(u, v)$ is a diametrical path, x_s is a pendent vertex. By Lemma 6, $d_{x_j} = 2$ and $d_{u_j} = 1$, where u_j is the neighbor of x_j different from y for $1 \le j \le s - 1$, and $u_1 = u$. So $2(2m-1) \ge \sum_{j=1}^{s-1} (d_{x_j} + d_{u_j}) + d_{x_s} + d_z + d_y + d_w \ge 3(s-1) + 1 + (s+1) + 2 + 1 = 4s + 2$, hence $s \le m - 1$. Consequently, $s \le m - 1$.

Let $T' = T - \{u, x\} \in T(2(m-1), m-1)$ and it is easily checked that $M - \{ux\}$ is a perfect matching of T'.

By the induction hypothesis, it is obvious that $M_1(T') \leq (m-1)^2 + 5(m-1) - 4$. Hence

$$M_1(T) \leq M_1(T') + d_x + d_u + d_y + d_x + \sum_{i=2}^s \left[(d_y + d_{x_i}) - (d_y - 1 + d_{x_i}) \right] + \left[(d_y + d_z) - (d_y - 1 + d_z) \right] \leq M_1(T') + 3 + (s+3) + s \leq (m-1)^2 + 5(m-1) - 4 + 6 + 2(m-1) = m^2 + 5m - 4,$$

equality occurs if and only if $M_1(T') = (m-1)^2 + 5(m-1) - 4$ and s = m-1 or equivalently, $T - \{u, x\} \cong T_{2(m-1),m-1}, yz \notin M$ and $d_y = m$, i.e. $T \cong T_{2m,m}$.

We can extend the result for the first Zagreb index of trees to the oriented trees.

Lemma 8. Let $T \in T(2m, m)$ with $m \ge 1$, $D \in \mathcal{O}(T)$. Then

$$M_1(D) \le \frac{1}{2}(m^2 + 5m - 4)$$

with equality if and only D is a sink-source orientation of $T_{2m,m}$.

Proof. Let $D \in \mathcal{O}(T)$, where $T \in T(2m, m)$. Since T is a bipartite graph, T has sink-source orientation, by Lemma 3.

From Lemma 4, $M_1(D) \leq \frac{1}{2}M_1(T)$, equality occurs if ond only if D is a sink-source orientation of T.

Hence, by Lemma 7,

$$\max\{M_1(D)|D \in \mathcal{O}(T), T \in T(2m,m)\} = \max\{\frac{1}{2}M_1(T)|T \in T(2m,m)\} = \frac{1}{2}M_1(T_{2m,m})$$

Consequently, $M_1(D) \leq \frac{1}{2}(m^2+5m-4)$, equality occurs if and only if D is a sink-source orientation of $T_{2m,m}$.

We give the maximum values of the first Zagreb index for orientations of two graph, which will be used in the following.

Lemma 9. Let $D \in \mathcal{O}(U_{4,2})$. Then

 $M_1(D) \le 8$

with equality if and only if $D \in \{U_{4,2}^{(1)}, U_{4,2}^{(2)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}\}$.



Figure 3: $D_i, i = 1, 2, \dots, 16.$

Proof. Let $D \in \mathcal{O}(U_{4,2})$. Since each $uv \in E(U_{4,2})$, uv has two orientations and $|E(U_{4,2})| = 4$, we have $|\mathcal{O}(U_{4,2})| = 2^4 = 16$. Note that $\mathcal{O}(U_{4,2}) = \{D_1, D_2, \dots, D_{16}\}$ (see Figure 3). Clearly, we have

$$M_1(D_1) = M_1(D_2) = M_1(D_{15}) = M_1(D_{16}) = 5$$
$$M_1(D_3) = M_1(D_6) = M_1(D_{11}) = M_1(D_{14}) = 6$$
$$M_1(D_7) = M_1(D_8) = M_1(D_9) = M_1(D_{10}) = 7$$
$$M_1(D_4) = M_1(D_5) = M_1(D_{12}) = M_1(D_{13}) = 8$$

Consequently, $M_1(D) \leq 8$, equality occurs if and only if $D \in \{D_4, D_5, D_{12}, D_{13}\}$ = $\{U_{4,2}^{(1)}, U_{4,2}^{(2)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}\}.$

Lemma 10. Let G_1 be the graph formed by attaching a pendent vertex to each vertex of a triangle. Let $D \in \mathcal{O}(G_1)$. Then

 $M_1(D) \le 13$

with equality if and only if $D \in \{D_{12}, D_{21}, D_{23}, D_{24}, D_{28}, D_{32}, D_{33}, D_{37}, D_{41}, D_{42}, D_{44}, D_{53}\}$ (see Figure 4).

Proof. Note that $\mathcal{O}(G_1) = \{D_i | i = 1, 2, \cdots, 64\}$ (see Figure 4).

Let u_i be a pendent vertex and v_i the unique neighbor of u_i in G_1 , where i = 1, 2, 3. Obviously, all digraphs in Figure 4 have $\{d_{u_i}^+ = 1, d_{u_i}^- = 0\}$ or $\{d_{u_i}^+ = 0, d_{u_i}^- = 1\}$, where i = 1, 2, 3. By Lemma 5,

$$M_{1}(D_{j}) = \frac{1}{2} \sum_{i=1}^{3} \left[(d_{D_{j}}^{+}(u_{i}))^{2} + (d_{D_{j}}^{-}(u_{i}))^{2} \right] + \frac{1}{2} \sum_{i=1}^{3} \left[(d_{D_{j}}^{+}(v_{i}))^{2} + (d_{D_{j}}^{-}v_{i})^{2} \right]$$
$$= \frac{1}{2} \left[3 + \sum_{i=1}^{3} \left[(d_{D_{j}}^{+}(v_{i}))^{2} + (d_{D_{j}}^{-}(v_{i}))^{2} \right] \right],$$



Figure 4: $D_i, i = 1, 2, \dots, 64$ in Lemma 10.

where $j = 1, 2, \dots, 64$. All digraphs in Figure 4 can be divided into three case:

Case 1. $\{d_{v_i}^+ = 2, d_{v_i}^- = 1\}$ or $\{d_{v_i}^+ = 1, d_{v_i}^- = 2\}$, where i = 1, 2, 3. This clearly implies that $M_1(D_2) = M_1(D_3) = M_1(D_4) = M_1(D_8) = M_1(D_7) = M_1(D_6)$ $= M_1(D_{13}) = M_1(D_{14}) = M_1(D_{15}) = M_1(D_{18}) = M_1(D_{25}) = M_1(D_{26})$ $= M_1(D_{29}) = M_1(D_{30}) = M_1(D_{35}) = M_1(D_{36}) = M_1(D_{39}) = M_1(D_{40})$ $= M_1(D_{47}) = M_1(D_{50}) = M_1(D_{51}) = M_1(D_{52}) = M_1(D_{57}) = M_1(D_{58})$ $= M_1(D_{59}) = M_1(D_{61}) = M_1(D_{62}) = M_1(D_{63}) = 9$

Case 2. There is a v_i which satisfy $\{d_{v_i}^+ = 3, d_{v_i}^- = 0\}$ or $\{d_{v_i}^+ = 0, d_{v_i}^- = 3\}$, says v_1 . $\{d_{v_i}^+ = 2, d_{v_i}^- = 1\}$ or $\{d_{v_i}^+ = 1, d_{v_i}^- = 2\}$, where i = 2, 3. This clearly implies that $M_1(D_1) = M_1(D_5) = M_1(D_9) = M_1(D_{10}) = M_1(D_{11}) = M_1(D_{16})$ $= M_1(D_{17}) = M_1(D_{19}) = M_1(D_{20}) = M_1(D_{22}) = M_1(D_{27}) = M_1(D_{31})$ $= M_1(D_{34}) = M_1(D_{38}) = M_1(D_{43}) = M_1(D_{45}) = M_1(D_{46}) = M_1(D_{48})$ $= M_1(D_{49}) = M_1(D_{54}) = M_1(D_{55}) = M_1(D_{56}) = M_1(D_{60}) = M_1(D_{64}) = 11$

Case 3. There are two v_i satisfy $\{d_{v_i}^+ = 3, d_{v_i}^- = 0\}$ or $\{d_{v_i}^+ = 0, d_{v_i}^- = 3\}$, say v_1 and v_2 . $\{d_{v_3}^+ = 1, d_{v_3}^- = 2\}$ or $\{d_{v_3}^+ = 2, d_{v_3}^- = 1\}$. This clearly implies that $M_1(D_{12}) = M_1(D_{21}) = M_1(D_{23}) = M_1(D_{24}) = M_1(D_{28}) = M_1(D_{32})$

 $= M_1(D_{33}) = M_1(D_{37}) = M_1(D_{41}) = M_1(D_{42}) = M_1(D_{44}) = M_1(D_{53}) = 13$

Consequantly, $M_1(D) \le 13$, equality occurs if and only if $D \in \{D_{12}, D_{21}, D_{23}, D_{24}, D_{28}, D_{32}, D_{33}, D_{37}, D_{41}, D_{42}, D_{44}, D_{53}\}$.

We are now ready to give a proof of Theorem 2.

Proof of Theorem 2.

Proof. We will prove by induction on m.

If m = 2, then either $G = C_4$ or $G = U_{4,2}$, and by Lemma 4, $D \in \mathcal{O}(C_4)$, $M_1(D) \leq \frac{1}{2}M_1(C_4) = 8 = \frac{1}{2}(2^2+7\times2-2)$, equality occurs if and only if D is a sink-source orientation of C_4 , i.e., $U_{4,2}^{(5)}$ or $U_{4,2}^{(6)}$. By Lemma 9, $D \in \mathcal{O}(U_{4,2})$, $M_1(D) \leq 8 = \frac{1}{2}[2^2+7\times2-2]$, equality occurs if and only if $D \in \{U_{4,2}^{(1)}, U_{4,2}^{(2)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}\}$. Consequently, $G \in U(4,2)$, $D \in \mathcal{O}(G)$, $M_1(D) \leq 8$, equality occurs if and only if $D \in \{U_{4,2}^{(1)}, U_{4,2}^{(2)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}, U_{4,2}^{(5)}, U_{4,2}^{(6)}\} = U_{4,2}^*$. The result holds.

If $m \geq 3$. Suppose that the result holds for all orientations of unicyclic graphs in U(2(m-1), m-1).

Let $G \in U(2m, m)$ with a perfect matching M. If $G = C_{2m}$, then $D \in \mathcal{O}(C_{2m})$, by Lemma 4 and $\frac{1}{2}(m^2 + 7m - 2) - 4m = \frac{1}{2}(m^2 - m - 2) = \frac{1}{2}[(m - \frac{1}{2})^2 - \frac{9}{4}] \ge 2 > 0$, $M_1(D) \le \frac{1}{2}M_1(C_{2m}) = 4m < \frac{1}{2}[m^2 + 7m - 2]$. The result holds.

Suppose that $G \neq C_{2m}$, we consider the following two cases.

Case 1. Suppose that G has a pendent vertex u whose unique neighbor v has degree two. Let $w \in N_G(v)$ and $w \neq u$. Obviously, $d_w \geq 2$. Let $N_G(w) = \{v_1, v_2, \dots, v_{s+1}\}$, where $s \geq 1$ and $v_1 = v$. Then M contains one of wv_i , $i = 2, 3, \dots, s+1$, say wv_2 . Since the s - 1 vertices v_3, \dots, v_{s+1} are M-saturated and at most two of them belong to the unicyclic component of $G - \{w\}$, we have $m \geq 2 + (s - 2) = s$. Then $G' = G - \{u, v\} \in$ U(2(m - 1), m - 1) and $M - \{uv\}$ is a perfect matching of G'. Let $D' \in \mathcal{O}(G')$ and $A(D') \bigcap A(D) = A(D')$, where $D \in \mathcal{O}(G)$.

By the induction hypothesis, it is obvious that $M_1(D') \leq \frac{1}{2}[(m-1)^2 + 7(m-1) - 2]$. If $uv \in A(D)$, then $\frac{1}{2}[d_D^+(u) + d_D^-(v)] \leq \frac{1}{2}[d_G(u) + d_G(v)]$. If $vu \in A(D)$, then $\frac{1}{2}[d_D^-(u) + d_D^+(v)] \leq \frac{1}{2}[d_G(u) + d_G(v)]$. Hence, $\max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} \leq \frac{1}{2}[d_G(u) + d_G(v)]$. Similarly to $vw \in A$ and $wv \in A$, and we have $\max\{\frac{1}{2}[d_D^+(v) + d_D^-(w)], \frac{1}{2}[d_D^-(v) + d_D^-(w)]\} \leq \frac{1}{2}[d_G(v) + d_D^-(w)]$.

If $vw \in A(D)$, then $d_D^-(w) = d_{D'}^-(w) + 1$, $d_D^+(w) = d_{D'}^+(w)$. Since $A(D') \cap A(D) = A(D')$, without lost of generality suppose that $d_D^+(v_i) = d_{D'}^+(v_i)$, where $i = 2, 3, \dots, d_D^-(w)$. $d_D^-(v_j) = d_{D'}^-(v_j)$, where $j = d_D^-(w) + 1, \dots, d_G(w)$. Consequently $d_D^+(v_i) + d_D^-(w) = d_{D'}^+(v_i) + d_{D'}^-(w) + 1$, where $i = 2, 3, \dots, d_D^-(w)$. $d_D^-(v_j) + d_D^+(w) = d_{D'}^-(v_j) + d_{D'}^+(w)$, where $j = d_D^-(w) + 1, \dots, d_G(w)$. Similarly to $wv \in A(D)$. Thus

$$\begin{split} M_{1}(D) \leqslant &M_{1}(D') + \max\{\frac{1}{2}[d_{D}^{+}(u) + d_{D}^{-}(v)], \frac{1}{2}[d_{D}^{-}(u) + d_{D}^{+}(v)]\} + \max\{\frac{1}{2}[d_{D}^{+}(w) + d_{D}^{-}(v)], \\ &\frac{1}{2}[d_{D}^{-}(w) + d_{D}^{+}(v)]\} + \frac{1}{2}\max\{\sum_{i=2}^{d_{D}^{+}(w)}[d_{D}^{-}(v_{i}) + d_{D}^{+}(w) - (d_{D'}^{-}(v_{i}) + d_{D'}^{+}(w))] \\ &+ \sum_{j=d_{D}^{+}(w)+1}^{d_{G}(w)}[d_{D}^{+}(v_{j}) + d_{D}^{-}(w) - (d_{D'}^{+}(v_{j}) + d_{D'}^{-}(w))], \sum_{i=2}^{d_{D}^{-}(w)}[d_{D}^{+}(v_{i}) + d_{D}^{-}(w) \\ &- (d_{D'}^{+}(v_{i}) + d_{D'}^{-}(w))] + \sum_{j=d_{D}^{-}(w)+1}^{d_{G}(w)}[d_{D}^{-}(v_{j}) + d_{D}^{+}(w) - (d_{D'}^{-}(v_{j}) + d_{D'}^{+}(w))] \} \end{split}$$

$$\leq M_{1}(D') + \frac{1}{2}[d_{G}(u) + d_{G}(v)] + \frac{1}{2}[d_{G}(w) + d_{G}(v)] + \frac{1}{2}\max\{d_{D}^{+}(w) - 1, d_{D}^{-}(w) - 1\}$$

$$\leq M_{1}(D') + \frac{1}{2}[d_{G}(u) + d_{G}(v)] + \frac{1}{2}[d_{G}(w) + d_{G}(v)] + \frac{1}{2}(d_{G}(w) - 1)$$

$$\leq M_{1}(D') + s + 3$$

$$\leq \frac{1}{2}[(m-1)^{2} + 7(m-1) - 2] + m + 3$$

$$= \frac{1}{2}[m^{2} + 7m - 2],$$

equality occurs if and only if $M_1(D') = \frac{1}{2} [(m-1)^2 + 7(m-1) - 2]$, $\max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} = \frac{1}{2}[d_G(u) + d_G(v)], \max\{\frac{1}{2}[d_D^+(w) + d_D^-(v)], \frac{1}{2}[d_D^-(w) + d_D^+(v)]\} = \frac{1}{2}[d_G(w) + d_G(v)], \frac{1}{2}\max\{[d_D^+(w) - 1], [d_D^-(w) - 1]\}\} = \frac{1}{2}[d_G(w) - 1] \text{ and } s = m,$ or equivalently, $D' \in U^*_{2(m-1),(m-1)}$ and $\{d_D^+(w) = m + 1, d_D^-(v) = d_G(v), d_D^+(u) = d_G(u)\}$ or $\{d_D^-(w) = m + 1, d_D^+(v) = d_G(v), d_D^-(u) = d_G(u)\}$, i.e. $D \in U^*_{2m,m}$. The result holds.

Case 2. Suppose that G has a pendent vertex u and $d_v \neq 2$ for $v \in N_G(u)$. $C = v_1 v_2 \dots v_t v_1$ denotes the unique cycle of G. Since M is a perfect matching of G, G - V(C) consists of isolated vertices.

Subcase 2.1. If each vertex of *C* is adjacent to a pendent vertex in *G*. Then $D \in \mathcal{O}(G)$. When $m \ge 4$, by Lemma 4 and $\frac{1}{2}[m^2+7m-2]-5m = \frac{1}{2}[m^2-3m-2] = \frac{1}{2}[(m-\frac{3}{2})^2-\frac{17}{8}] > 0$, we have $M_1(D) \le \frac{1}{2}M_1(G) = 5m < \frac{1}{2}[m^2+7m-2]$. When m = 3, by Lemma 10, $M_1(D) \le 13 < 14 = \frac{1}{2}(3^2+7\times 3-2)$. The result holds.

Subcase 2.2. Suppose that there is at least one vertex of degree two on C. Obviously, $d_{v_1} = 2 \text{ or } 3$. Without lost of generality suppose that $d_{v_2} = 3$ and $d_{v_3} = 2$. Let $u_2 \in N_G(v_2)$ and $d_{u_2} = 1$. Since $v_2u_2 \in M$ and v_3 is M-saturated, we have $v_3v_4 \in M$ and thus $d_{v_4} = 2$. Let $T' = G - \{v_2, u_2\}$. Then $T' \in T(2(m-1), m-1)$ and $M - \{u_2v_2\}$ is a perfect matching of T'.

By Lemma 8, $T' \in T(2(m-1), m-1)$, $D' \in \mathcal{O}(T')$ and $A(D') \cap A(D) = A(D')$, where $D \in \mathcal{O}(G)$. Then $M_1(D') \leq \frac{1}{2}[(m-1)^2 + 5(m-1) - 4]$. Thus

$$\begin{split} M_1(D) &\leq M_1(D') + max\{\frac{1}{2}[d_D^+(v_2) + d_D^-(u_2)], \frac{1}{2}[d_D^-(v_2) + d_D^+(u_2)]\} + max\{\frac{1}{2}[d_D^+(v_2) + d_D^-(v_2)], \frac{1}{2}[d_D^-(v_2) + d_D^+(v_3)]\} + \frac{1}{2}max\{d_D^+(v_1) - d_D^-(v_1), \frac{1}{2}[d_D^-(v_2) + d_D^+(v_3)]\} + \frac{1}{2}max\{d_D^+(v_1) - 1, d_D^-(v_1) - 1\} + \frac{1}{2}max\{d_D^+(v_3) - 1, d_D^-(v_3) - 1\} \leq M_1(D') + \frac{1}{2}[d_G(v_2) + d_G(u_2)] + \frac{1}{2}[d_G(v_2) + d_G(v_3)] + \frac{1}{2}(d_G(v_1) - 1) + \frac{1}{2}(d_G(v_3) - 1) \leq \frac{1}{2}[(m-1)^2 + 5(m-1) - 4 + 8 + 10] = \frac{1}{2}[m^2 + 3m + 10]. \end{split}$$

Since $\frac{1}{2}[m^2 + 7m - 2] - \frac{1}{2}[m^2 + 3m + 10] = \frac{1}{2}[4m - 12] \ge 0, M_1(D) \le \frac{1}{2}[m^2 + 3m + 10] \le \frac{1}{2}[m^2 + 7m - 2]$ with equality if and only if $D \in \{U_{6,3}^{(5)}, U_{6,3}^{(6)}\}$. Consequently, the result holds.

4 Proof of Theorem 1

In this section we give a proof of Theorem 1. For this we need the following results:

Lemma 11. [10] Let $G \in U(n,m)$ with $G \neq C_n$, where n > 2m. Then there is a maximum matching M of G and a pendent vertex u such that is not M-saturated.

Lemma 12. Let n and m be integers with $2 \le m \le \lfloor \frac{n}{2} \rfloor$ and n > 2m. Then

$$\frac{1}{2}\left[n^2 + (-2m+3)n + m^2 + m - 2\right] > 2m$$

Proof. Let

$$f(n,m) = \frac{1}{2} \left[n^2 + (-2m+3)n + m^2 + m - 2 \right] - 2n$$

then

$$\frac{\partial f}{\partial m} = \frac{1}{2}(2m+1-2n) < 0$$

When n is even, $\lfloor \frac{n}{2} \rfloor = \frac{n}{2}$. Since n > 2m i.e., $m < \frac{n}{2}, 2 \le m < \frac{n}{2}$. Hence $f(n,m) \ge f(n, \frac{n-2}{2})$. Let $h(n) = f(n, \frac{n-2}{2}) = \frac{1}{8}n^2 + \frac{1}{4}n - 1$. Since $h'(n) = \frac{n}{4} + \frac{1}{4} > 0$, $h(n) \ge h(5) = \frac{27}{8} > 0$. Consequently, $f(n,m) \ge f(n, \frac{n}{2} - 1) > 0$, i.e. $\frac{1}{2} [n^2 + (-2m + 3)n + m^2 + m - 2] > 2n$.

When n is odd, $\lfloor \frac{n}{2} \rfloor = \frac{n-1}{2}$. Since $f(n, \frac{n-1}{2}) = \frac{1}{2} \left[n^2 + (4-n)n + \frac{1}{4}(n-1)^2 + \frac{n-1}{2} - 2 \right] - 2n = -\frac{9}{8} + \frac{n^2}{8}$ and $n \ge 2m \ge 4$, $f(n, \frac{n-1}{2}) \ge 2 - \frac{8}{9} > 0$. Consequently, the results holds. \Box

We are now ready to give a proof of Theorem 1. **Proof of Theorem 1**.

Proof. We will prove by induction on n.

If n = 2m, by Theorem 1, the result holds.

If n > 2m. Suppose that the result holds for orientations of all unicyclic graphs on less than n vertices.

Let $G \in U(n,m)$. If $G = C_n$, then $D \in \mathcal{O}(C_n)$, by Lemma 4 and Lemma 12, $M_1(D) \leq \frac{M_1(C_n)}{2} = 2n < \frac{1}{2} [n^2 + (-2m+3)n + m^2 + m - 2]$. The result holds. If $G \neq C_n$. By Lemma 11, G has a maximum matching M and a pendent vertex u such that u is not M-saturated. Then $G' = G - \{u\} \in U(n-1,m)$. Let $D' \in \mathcal{O}(G')$ and $A(D') \cap A(D) = A(D')$.

By the induction hypothesis, it is obvious that

$$M_1(D') \le \frac{1}{2} \left[(n-1)^2 + (-2m+3)(n-1) + m^2 + m - 2 \right].$$

Let $v \in N_G(u)$ and $N_G(v) = \{u_1, u_2, \dots, u_{s+1}\}$, where $s \ge 1$ and $u_1 = u$. Since M contains at most one of the edges vu_i for $i = 2, 3, \dots, s+1$ and there are n - m edges of G outside M, it is obvious that $s \le n - m$.

If $uv \in A(D)$, then $\frac{1}{2}[d_D^+(u) + d_D^-(v)] \leq \frac{1}{2}[d_G(u) + d_G(v)]$. If $vu \in A(D)$, then $\frac{1}{2}[d_D^-(u) + d_D^+(v)] \leq \frac{1}{2}[d_G(u) + d_G(v)]$. Hence, $\max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} \leq \frac{1}{2}[d_G(u) + d_G(v)]$.

If $uv \in A(D)$, then $d_D^-(v) = d_{D'}^-(v) + 1$, $d_D^+(v) = d_{D'}^+(v)$. Since $A(D') \cap A(D) = A(D')$, without lost of generality suppose that $d_D^+(u_i) = d_{D'}^+(u_i)$, where $i = 2, \dots, d_D^-(v)$; $d_D^-(u_j) = d_{D'}^-(u_j)$, where $j = d_D^-(v) + 1, \dots, d_G(v)$, we have $d_D^+(u_i) + d_D^-(v) = d_{D'}^+(u_i) + d_{D'}^-(v) + 1$, where $i = 2, \dots, d_D^-(v)$; $d_D^-(u_j) + d_D^+(v) = d_{D'}^-(u_j) + d_{D'}^+(v)$, where $j = d_D^-(v) + 1, \dots, d_G(v)$.

Similarly to $vu \in A(D)$. Thus

$$\begin{split} M_1(D) \leqslant &M_1(D') + \max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} + \max\{\frac{1}{2}\sum_{i=2}^{d_D^+(v)}[d_D^-(u_i) \\ &+ d_D^+(v) - (d_{D'}^-(u_i) + d_{D'}^+(v))] + \frac{1}{2}\sum_{j=d_D^+(v)+1}^{d_G(v)}[d_D^+(u_j) + d_D^-(v) - (d_{D'}^+(u_j) + d_{D'}^-(v))], \\ &\frac{1}{2}\sum_{i=2}^{d_D^-(v)}[d_D^+(u_i) + d_D^-(v) - (d_{D'}^+(u_i) + d_{D'}^-(v))] + \frac{1}{2}\sum_{j=d_D^-(v)+1}^{d_G(v)}[d_D^-(u_j) + d_D^+(v) \\ &- (d_{D'}^-(u_j) + d_{D'}^+(v))]\} \\ &\leqslant M_1(D') + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}\max\{d_D^+(v) - 1, d_D^-(v) - 1\} \\ &\leqslant M_1(D') + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}(d_G(v) - 1) \\ &\leqslant M_1(D') + s + 1 \\ &\leqslant \frac{1}{2}\left[(n-1)^2 + (-2m+3)(n-1) + m^2 + m - 2\right] + n - m + 1 \\ &= \frac{1}{2}\left[n^2 + (-2m+3)n + m^2 + m - 2\right] \end{split}$$

with equality if and only if $M_1(D') = \frac{1}{2} [(n-1)^2 + (-2m+3)(n-1) + m^2 + m - 2],$ $\max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} = \frac{1}{2}[d_G(u) + d_G(v)], \frac{1}{2}\max\{[d_D^+(v) - 1], [d_D^-(v) - 1],$ 1]} = $\frac{1}{2}[d_G(v)-1]$ and s = n-m, or equivalently, $D' \in U^*_{n-1,m}$ and $\{d^+_D(u) = d_G(u), d^-_D(v) = d_G(v)\}$ or $\{d^+_D(v) = d_G(v), d^-_D(u) = d_G(u)\}$, i.e. $D \in U^*_{n,m}$. The result holds.

Acknowledgment. This work is supported by the Hunan Provincial Natural Science Foundation of China (2020JJ4423), the Department of Education of Hunan Province (19A318) and the National Natural Science Foundation of China (11971164).

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