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. $d_v^-$) 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 $m$ ($2 \leq m \leq \lfloor \frac{n}{2} \rfloor$).

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 $d_G(v) = |N_G(v)|$ 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 $G$ obtained by deleting the vertices of $W$ and the edges incident with them. A matching $M$ of 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 $V$ of 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 $d_u^+$ (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 $O(G)$ be the set of all orientations of $G$. $D \in O(G)$, if $d_u^+ = 0$ or $d_u^- = 0$ for any $u \in V(D)$, then $D$ is 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 $OT(n)$, the set of all oriented trees with $n$ vertices. Also, the authors given the extremal values of the Randić index over $O(P_n), O(C_n)$ and $O(H_d)$, 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 $OT(n)$ and $O(G)$, respectively. But the maximum value of $AZ$ over $OT(n)$ 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 $m$ ($2 \leq m \leq \lfloor \frac{n}{2} \rfloor$), and we state the results as follows:

Let $n$ and $m$ be integers and $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$, $U(n, m)$ the class of unicyclic graphs on $n$
vertices with matching number $m$, and $U_{n,m}$ the graph formed by attaching $n - 2m + 1$ pendent vertices and $m - 2$ paths of length 2 to a (common) vertex of a triangle. Let $U^{(1)}_{n,m}, U^{(2)}_{n,m}, U^{(3)}_{n,m}, U^{(4)}_{n,m}$ be four orientations of $U_{n,m}$ (see Figure 1). Obviously, $U_{n,m} \in U(n, m)$. Let $C_n$ be the cycle with $n$ vertices. $U^*_n = \{U^{(1)}_{4,2}, U^{(2)}_{4,2}, U^{(3)}_{4,2}, U^{(5)}_{4,2}, U^{(6)}_{4,2}\}$, where $U^{(5)}_{4,2}$ and $U^{(6)}_{4,2}$ are the sink-source orientations of $C_4$. $U^*_6 = \{U^{(1)}_{6,3}, U^{(2)}_{6,3}, U^{(3)}_{6,3}, U^{(4)}_{6,3}, U^{(5)}_{6,3}, U^{(6)}_{6,3}\}$, where $U^{(5)}_{6,3}$ and $U^{(6)}_{6,3}$ are the sink-source orientations of the graph formed by attaching two pendant vertices to two adjacent vertices of $C_4$. $U^*_{n,m} = \{U^{(1)}_{n,m}, U^{(2)}_{n,m}, U^{(3)}_{n,m}, U^{(4)}_{n,m}\}$, where $(n, m) \neq (4, 2), (6, 3)$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Four orientations of $U_{n,m} : U^{(1)}_{n,m}, U^{(2)}_{n,m}, U^{(3)}_{n,m}, U^{(4)}_{n,m}$.}
\end{figure}

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

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

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 $m \geq 2$, $D \in \mathcal{O}(G)$. Then

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

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 $m$ ($2 \leq m \leq \lfloor \frac{n}{2} \rfloor$).

## 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

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

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 $d_u \geq d_u^+$ and $d_v \geq d_v^-$, where $u, v \in V$. Then $d_u^+ + d_v^- \leq d_u + d_v$. Hence

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

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 $d_v^- = 0$, 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, $d_u \geq d_u^+$ and $d_v \geq d_v^-$, then $d_u + d_v \geq d_u^+ + d_v^-$ 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 $d_u^w = 0$ or $d_v^w = 0$ for any $w \in V$. $\Box$

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

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

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

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

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 $m$ ($m \geq 1$).

Let $n$ and $m$ be integers and $1 \leq m \leq \lfloor \frac{n}{2} \rfloor$. $T(n, m)$ 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 \( T_{n,m} \).](image)

**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 \( m \geq 1 \). Then

\[
M_1(T) \leq m^2 + 5m - 4
\]

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 \( P_T(u,v) = ux_1y \cdots \) a diametrical path in \( T \). Then \( z \neq v \). Let \( N_T(y) = \{x_1, x_2, \ldots, x_{s+1}\} \) 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 \( 1 \leq i \leq s \), and \( u_1 = u \). So

\[
2(2m-1) \geq \sum_{i=1}^{s} (d_{x_i}+d_{u_i}) + d_y + d_z + d_v \geq 3s + (s+1) + 2 + 1 > 4s + 2, \text{ hence } s < m - 1.
\]

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 \( 2 \leq i \leq s \), 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 \( 1 \leq j \leq s-1 \), and \( u_1 = u \). So

\[
2(2m-1) \geq \sum_{j=1}^{s-1} (d_{x_j}+d_{u_j}) + d_{x_s} + d_z + d_y + d_w \geq 3(s-1) + 1 + (s+1) + 2 + 1 = 4s + 2, \text{ hence } s \leq m - 1.
\]

Consequently, \( s \leq m - 1 \).

Let \( T' = T \setminus \{u,x\} \in T(2(m-1),m-1) \) and it is easily checked that \( M \setminus \{ux\} \) 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

\[
M_1(T) \leq M_1(T') + d_x + d_u + d_y + d_x + \sum_{i=2}^{s} [(d_y + d_z) - (d_y - 1 + d_x)]
\]
\[
+ [(d_y + d_z) - (d_y - 1 + d_z)]
\]
\[
\leq M_1(T') + 3 + (s + 3) + s
\]
\[
\leq (m - 1)^2 + 5(m - 1) - 4 + 6 + 2(m - 1)
\]
\[
= m^2 + 5m - 4,
\]
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. \( T \cong T_{2m,m} \). \hfill \qed

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 \( m \geq 1 \), \( D \in \mathcal{O}(T) \). Then

\[
M_1(D) \leq \frac{1}{2}(m^2 + 5m - 4)
\]

with equality if and only if \( D \) 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 and 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 \( T_{2m,m} \). \hfill \qed

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

\[
M_1(D) \leq 8
\]

with equality if and only if \( D \in \{U^{(1)}_{4,2}, U^{(2)}_{4,2}, U^{(3)}_{4,2}, U^{(4)}_{4,2}\} \).
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 \( \mathcal{O}(U_{4,2}) = \{D_1, D_2, \cdots, D_{16}\} \) (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 \( D \in \{D_4, D_5, D_{12}, D_{13}\} \) = \( \{U^{(1)}_{4,2}, U^{(2)}_{4,2}, U^{(3)}_{4,2}, U^{(4)}_{4,2}\} \).

\[ \square \]

**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

\[
M_1(D) \leq 13
\]

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

\[
M_1(D_j) = \frac{1}{2} \sum_{i=1}^{3} \left[ (d_{D_j}^+(u_i))^2 + (d_{D_j}^-(u_i))^2 \right] + \frac{1}{2} \sum_{i=1}^{3} \left[ (d_{D_j}^+(v_i))^2 + (d_{D_j}^-(v_i))^2 \right] \\
= \frac{1}{2} \left[ 3 + \sum_{i=1}^{3} \left[ (d_{D_j}^+(v_i))^2 + (d_{D_j}^-(v_i))^2 \right] \right],
\]
where \( j = 1, 2, \ldots, 64 \). 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 \( v_1 \). \( \{d^+_{v_1} = 2, d^-_{v_1} = 1\} \) or \( \{d^+_{v_1} = 1, d^-_{v_1} = 2\} \), where \( i = 2, 3 \). This clearly implies that
\( M_1(D_1) = M_1(D_5) = M_1(D_8) = M_1(D_{10}) = M_1(D_{11}) = M_1(D_{16}) \)
\( = M_1(D_{17}) = M_1(D_{19}) = M_1(D_{20}) = M_1(D_{22}) = M_1(D_{27}) = M_1(D_{31}) \)
\( = M_1(D_{34}) = M_1(D_{38}) = M_1(D_{43}) = M_1(D_{45}) = M_1(D_{46}) = M_1(D_{48}) \)
\( = M_1(D_{49}) = M_1(D_{54}) = M_1(D_{55}) = M_1(D_{56}) = M_1(D_{60}) = M_1(D_{64}) = 11 \)

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 \( v_2 \). \( \{d^+_{v_1} = 1, d^-_{v_1} = 2\} \) or \( \{d^+_{v_1} = 2, d^-_{v_1} = 1\} \). This clearly implies that \( M_1(D_{12}) = M_1(D_{21}) = M_1(D_{23}) = M_1(D_{24}) = M_1(D_{28}) = M_1(D_{32}) \)
\( = M_1(D_{33}) = M_1(D_{37}) = M_1(D_{41}) = M_1(D_{42}) = M_1(D_{44}) = M_1(D_{53}) = 13 \)

Consequently, \( M_1(D) \leq 13 \), equality occurs if and only if \( D \in \{D_{12}, D_{21}, D_{23}, D_{24}, D_{28}, D_{32}, D_{33}, D_{37}, D_{41}, D_{42}, D_{44}, D_{53}\} \).
The result holds.

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, \( D \in \mathcal{O}(C_4) \), \( M_1(D) \leq \frac{1}{2}M_1(C_4) = 8 = \frac{1}{2}(2^2 + 7 \times 2 - 2) \), 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 5, \( D \in \mathcal{O}(U_{4,2}) \), \( M_1(D) \leq 8 = \frac{1}{2}[2^2 + 7 \times 2 - 2] \), 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 \( D \in \{ U_{4,2}^{(1)}, U_{4,2}^{(2)}, U_{4,2}^{(3)}, U_{4,2}^{(4)}, U_{4,2}^{(5)} \} = U_{4,2}^* \).

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 \( \frac{1}{2}(m^2 + 7m - 2) - 4m = \frac{1}{2}(m^2 - m - 2) = \frac{1}{2}[(m - \frac{1}{2})^2 - \frac{9}{4}] \geq 2 > 0 \), \( M_1(D) \leq \frac{1}{2}M_1(C_{2m}) = 4m < \frac{1}{2}[m^2 + 7m - 2] \). The result holds.

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

Case 1. Suppose that \( G \) has a pendant 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 \( N_G(w) = \{ v_1, v_2, \ldots, v_{s+1} \} \), where \( s \geq 1 \) and \( v_1 = v \). Then \( M \) contains one of \( wv_i, i = 2, 3, \ldots, s + 1 \), say \( wv_2 \). Since the \( s - 1 \) vertices \( v_3, \ldots, v_{s+1} \) 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 \( M - \{ wv \} \) is a perfect matching of \( G' \). Let \( D' \in \mathcal{O}(G') \) and \( A(D') \cap A(D) = A(D') \), 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 \( wv \in A(D) \), then \( \frac{1}{2}[d_D'(u) + d_D'(v)] \leq \frac{1}{2}[d_G(u) + d_G(v)] \). If \( uv \in A(D) \), then \( \frac{1}{2}[d_D(u) + d_D(v)] \leq \frac{1}{2}[d_G(u) + d_G(v)] \). 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 \( wv \in A \) and \( uv \in A \), and we have \( \max\{ \frac{1}{2}[d_D'(u) + d_D'(v)], \frac{1}{2}[d_D(u) + d_D(v)] \} \). If \( wv \in A(D) \), then \( d_D'(w) = d_G'(w) + 1, d_D'(w) = d_G'(w) \). Since \( A(D') \cap A(D) = A(D') \), without lost of generality suppose that \( d_D'(v_i) = d_G'(v_i) \), where \( i = 2, 3, \ldots, d_D'(w) \).

Thus, \( d_D'(v) = d_G'(v) = d_D'(v_1) + d_D'(v_2) + \cdots + d_D'(v_s) \). Consequently \( d_D'(v_i) + d_D'(w) = d_G'(v_i) + d_G'(w) + 1, \) where \( i = 2, 3, \ldots, d_D'(w) \).

Similarly to \( wv \in A(D) \). Thus
$$M_1(D) \leq M_1(D') + \max\left\{ \frac{1}{2}[d_D(u) + d_D^+(v)], \frac{1}{2}[d_D(u) + d_D^+(v)] \right\} + \max\left\{ \frac{1}{2}[d_D^+(w) + d_D^-(w)], \frac{1}{2}[d_D^+(w) + d_D^-(w)] \right\}$$

$$= \frac{1}{2}[d_D^+(w) + d_D^+(v)] + \frac{1}{2} \max\left\{ \sum_{i=2}^{d_G(w)} [d_D(v_i) + d_D^+(w) - (d_D^-(v_i) + d_D^+(w))] \right\}$$

$$+ \sum_{j=d_D^+(w)+1}^{d_G(w)} [d_D^+(v_j) + d_D^+(w) - (d_D^-(v_j) + d_D^+(w))] + \max\left\{ \sum_{i=2}^{d_G(w)} [d_D^+(v_i) + d_D^+(w)] \right\}$$

$$- (d_D^-(v_i) + d_D^+(w))] + \max\left\{ \sum_{i=2}^{d_G(w)} [d_D^+(v_i) + d_D^+(w) - (d_D^-(v_i) + d_D^+(w))] \right\}$$

$$\leq M_1(D') + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2} \max\{d_D^+(w) - 1, d_D^-(w) - 1\}$$

$$\leq M_1(D') + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}(d_G(w) - 1)$$

$$\leq M_1(D') + s + 3$$

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

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

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\{\frac{1}{2}[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 \(d_u \neq 2\) for \(v \in N_G(u).\) \(C = v_1v_2...v_tv_1\) 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 \(D \in O(G).\)

When \(m \geq 4,\) by Lemma and \(\frac{1}{2}[m^2+7m-2]-5m = \frac{1}{2}[m^2-3m-2] = \frac{1}{2}[m^2-3m^2-\frac{17}{8}] > 0,\)

we have \(M_1(D) \leq \frac{1}{2}M_1(G) = 5m < \frac{1}{2}[m^2+7m-2].\) When \(m = 3,\) by Lemma \(M_1(D) \leq 13 < 14 = \frac{1}{2}(3^2 + 7 \times 3 - 2).\) The result holds.

Subcase 2.2. Suppose that there is at least one vertex of degree two on \(C.\) Obviously, \(d_{v_1} = 2\) 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 \(T' \in T(2(m-1), m-1), D' \in O(T')\) and \(A(D') \cap A(D) = A(D'),\) where \(D \in O(G).\) Then \(M_1(D') \leq \frac{1}{2}[(m-1)^2 + 5(m-1) - 4].\) Thus
\[ M_1(D) \leq M_1(D') + \max\left\{ \frac{1}{2}[d_D^+(v_2) + d_D^+(u_2)], \frac{1}{2}[d_D^-(v_2) + d_D^-(u_2)] \right\} + \max\left\{ \frac{1}{2}[d_D^+(v_2) + d_D^+(v_1)], \frac{1}{2}[d_D^-(v_2) + d_D^-(v_1)] \right\} + \max\left\{ \frac{1}{2}[d_D^+(v_2) + d_D^+(v_3)], \frac{1}{2}[d_D^-(v_2) + d_D^-(v_3)] \right\} + \frac{1}{2} \max\left\{ d_D^-(v_1) - 1, d_D^+(v_1) - 1 \right\} + \frac{1}{2} \max\left\{ d_D^+(v_3) - 1, d_D^-(v_3) - 1 \right\} \leq M_1(D') + \frac{1}{2}[d_G(v_2) + d_G(u_2)] + \frac{1}{2}[d_G(v_2) + d_G(v_1)] + \frac{1}{2}[d_G(v_2) + d_G(v_3)] + \frac{1}{2}(d_G(v_1) - 1) + \frac{1}{2}(d_G(v_3) - 1) \leq \frac{1}{2}[(m - 1)^2 + 5(m - 1) - 4 + 8 + 10] = \frac{1}{2}[m^2 + 3m + 10]. \]

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

\[ \square \]

### 4 Proof of Theorem 1

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

**Lemma 11.** 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 \( 2 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor \) and \( n > 2m \). Then

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

**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, \( \left\lfloor \frac{n}{2} \right\rfloor = \frac{n}{2} \). Since \( n > 2m \) i.e., \( m < \frac{n}{2} \), \( 2 \leq m < \frac{n}{2} \). Hence \( f(n, m) \geq f(n, \frac{n-2}{2}) \). Let \( h(n) = f(n, \frac{n-2}{2}) = \frac{1}{8}n^2 + \frac{1}{4}n - 1 \). Since \( h'(n) = \frac{n}{4} + \frac{1}{4} > 0 \), \( h(n) \geq h(5) = \frac{27}{8} > 0 \). Consequently, \( f(n, m) \geq f(n, \frac{n-2}{2}) > 0 \), i.e. \( \frac{1}{2} \left[ n^2 + (-2m + 3)n + m^2 + m - 2 \right] > 2n \).

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

\[ \square \]

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. \( M_1(D) \leq \frac{M_1(C_n)}{2} = 2n < \frac{1}{2} \left[ n^2 + (-2m + 3)n + m^2 + m - 2 \right] \). 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

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

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

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, $\max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} = \frac{1}{2}[d_G(u) + d_G(v)]$.

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 $i = 2, \ldots, d_D^+(v)$; $d_D^-(u_i) = d_D^-(u_j)$, where $j = d_D^-(v) + 1, \ldots, d_G(v)$, we have $d_D^+(u_i) + d_D^-(v) = d_D^+(u_i) + d_D^-(v) + 1$, where $i = 2, \ldots, d_D^+(v)$; $d_D^+(u_i) + d_D^-(v) = d_D^+(u_j) + d_D^-(v)$, where $j = d_D^-(v) + 1, \ldots, d_G(v)$.

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

$$M_1(D) \leq M_1(D') + \max\{\frac{1}{2}[d_D^+(u) + d_D^-(v)], \frac{1}{2}[d_D^-(u) + d_D^+(v)]\} + \frac{1}{2} \sum_{i=2}^{d_G(v)} [d_D^+(u_i) + d_D^-(v) - (d_D^+(u_i) + d_D^-(v))],$$

$$\frac{1}{2} \sum_{i=2}^{d_G(v)} [d_D^+(u_i) + d_D^-(v) - (d_D^+(u_i) + d_D^-(v))],$$

$$\frac{1}{2} \sum_{j=d_D^-(v)+1}^{d_G(v)} [d_D^+(u_j) + d_D^-(v) - (d_D^+(u_j) + d_D^-(v))],$$

$$\frac{1}{2} \sum_{j=d_D^-(v)+1}^{d_G(v)} [d_D^+(u_j) + d_D^-(v) - (d_D^+(u_j) + d_D^-(v))],$$

$$M_1(D') + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}\max\{d_D^+(v) - 1, d_D^-(v) - 1\}$$

$$\leq M_1(D') + \frac{1}{2}[d_G(u) + d_G(v)] + \frac{1}{2}\max\{d_G(v) - 1\}$$

$$\leq M_1(D') + \frac{1}{2}(n - 1)^2 + (-2m + 3)(n - 1) + m^2 + m - 2] + n - m + 1$$

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

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

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**References**

[1] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total \( \pi \)-electronenergy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.

[2] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecularorbitals. XII. Acyclic polyenes, J. Chem. Phys. 62 (1975) 3399-3405.

[3] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: Extremal results and bounds, MATCH Commun. Math. Comput. Chem. 80 (2018) 5-84.

[4] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, MATCH Commun. Math. Comput. Chem. 78 (2017) 17-100.

[5] K. C. Das, Sharp bounds for the sum of the squares of degrees of a graph, Kragujevac J. Math. 25 (2003) 31-49.

[6] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, Discr. Math. 285 (2004) 57-66.

[7] K. C. Das, On comparing Zagreb indices of graphs, MATCH Commun. Math. Comput. Chem. 63 (2010) 433-440.

[8] K. C. Das, I. Gutman, B. Zhou, New upper bounds on Zagreb indices, J. Math. Chem. 46 (2009) 514-521.

[9] B. Zhou, Remarks on Zagreb indices, MATCH Commun. Math. Comput. Chem. 57 (2007) 591-596.

[10] A. Yu, F. Tian, On the spectral radius of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 51 (2004) 97-109.

[11] S. Nikolić, G. Kovačević, A. Milčević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta. 76 (2) (2003) 113-124.

[12] J. Monsalve, J. Rada, Vertex-degree based topological indices of digraphs, Discrete Appl. Math. 295 (2021) 13-24.

[13] J. Monsalve, J. Rada, Oriented bipartite graphs with minimal trace norm, Linear Multilinear A. 67 (6) (2019) 1121-1131.
[14] J. Monsalve, J. Rada, Sharp upper and lower bounds of VDB topological indices of digraphs, Symmetry, 13 (2021) 1903-1904.

[15] W. Luo, B. Zhou, On the irregularity of trees and unicyclic graphs with given matching number, Util. Math. 83 (2010) 141-148.