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Research article

Extremal graphs with maximum complementary second Zagreb index

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Abstract: The complementary second Zagreb index of a graph G is defined as $cM_2(G) = \sum_{uv\in E(G)} |d_G(u)^2 - d_G(v)^2|$. In this paper, we prove that a graph having maximum complementary second Zagreb index among all graphs of order n is isomorphic to $K_m \vee \overline{K_{n-m}}$ for some $1 \le m < \lceil \frac{n}{2} \rceil$, confirming a conjecture of Furtula and Oz.

Keywords: complementary second Zagreb index; extremal graph; mixed graph; orientation; cM_2-maximal
Mathematics Subject Classification: 05C35, 05C92

1. Introduction

All graphs, digraphs, and mixed graphs in this paper are considered to be simple; that is, they have no loops or parallel edges or arcs.

Let F be a mixed graph with vertex set $V(F)$, edge set $E(F)$, and arc set $A(F)$. Since a graph or digraph can be seen as a special mixed graph with an empty arc set or empty edge set, respectively, the following definitions are claimed only for mixed graphs.

For $X \subseteq V(F)$, denote by $F[X]$ the mixed graph with vertex set X and edge set and arc set consisting of edges and arcs in F with both of their end-vertices in X, respectively. For $u \in V(F)$, denote by $N_F^+(u)$, $N_F^-(u)$, and $N_F(u)$ the set of arcs with u as their tails, the set of arcs with u as their heads, and the set of all edges and arcs incident with u, respectively. Denote $d_F^+(u) := |N_F^+(u)|$, $d_F^-(u) := |N_F^-(u)|$ and $d_F(u) := |N_F(u)|$. For an edge set E_0 and arc set A_0, denote by $F \pm E_0$ ($F \pm A_0$) the mixed graph by adding to F or deleting in F all edges in E_0 (all arcs in A_0), respectively. For simplicity, if E_0 or A_0 is a singleton set, say $\{a_0\}$, then we always write $F \pm a_0$ rather than $F \pm \{a_0\}$. Let G and H be graphs. Denote by $\overline{G}$ the graph with vertex set $V(G)$ and edge set consisting of pairs of nonadjacent vertices of G. Denote by $G \vee H$ the graph by starting with a disjoint union of two graphs, G and H, and adding edges joining every vertex of G to every vertex of H. For all notations and terminology used, but not defined here, we refer to the textbook [1].

In the field of chemical molecular graphs, the atoms are represented by vertices and the bonds by edges that capture the structural essence of compounds. The numerical representation of the molecule graph can be mathematically deduced as a single number, usually called a graph invariant or topological index [5, 9, 10]. The first Zagreb index $M_1(G)$ is the sum of the square of degrees of all the atoms, and the second Zagreb index $M_2(G)$ is the sum over all bonds of the product of the vertex degrees of the two adjacent atoms; that is, for any graph $G = (V, E)$ with vertex set $V(G)$ and edge set $E(G)$,

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

For recent work on Zagreb indices, the readers are referred to [2, 11, 12].

Furtula and Oz [3] presented a novel way of contemplating the concept of geometrical degree-based topological indices. By applying this approach, they defined the so-called "complementary second Zagreb index" of a graph G, which is defined by

$$cM_2(G) := \sum_{uv \in E(G)} |d_G(u)^2 - d_G(v)^2|.$$

As observed in [3], this index is not put forward here for the first time. It was introduced and reintroduced in several recent and unrelated papers, which resulted in several names for this index, such as the nano Zagreb index [7], the minus-F index [8], the modified Albertson index [16], and the first Sombor index [4, 6, 15].

Furtula and Oz [3] conjectured that the graph having maximum complementary second Zagreb index among all graphs of order n is isomorphic to $K_m \vee \overline{K_{n-m}}$ for some $1 \leq m < \frac{n}{2}$. Recently, Saber, Alraqad, Ali, Alanazi, and Raza [14] established results that support the conjecture under consideration for characteristics of the maximum or minimum degree of the extremal graph and for bidegreed and tridegreed graphs. In this paper, we give a complete proof of this conjecture.

Theorem 1. *The graph having maximum complementary second Zagreb index among all graphs of order $n(\geq 3)$ is isomorphic to $K_m \vee \overline{K_{n-m}}$ for some $1 \leq m \leq n$.*

Theorem 2. *If m_n is such that $cM_2(K_{m_n} \vee \overline{K_{n-m_n}})$ reaches the maximum complementary second Zagreb index among all graphs of order n, then,*

(i) $\dfrac{m_n}{n} < \dfrac{1}{2}$,

(ii) $\lim\limits_{n \to \infty} \dfrac{m_n}{n} = \dfrac{\sqrt{17} - 1}{8}$.

2. Preliminaries

Let $G = (V, E)$ be an undirected graph with n vertices, and F be the mixed graph obtained by orienting some edges in G as follows:
(i) $\overrightarrow{uv} \in A(F)$ if $uv \in E(G)$ and $d_G(u) > d_G(v)$,
(ii) $uv \in E(F)$ if $uv \in E(G)$ and $d_G(u) = d_G(v)$.

Denote by X and Y the set of vertices satisfying $d^+_F(u) \geq d^-_F(u)$ and $d^+_F(u) < d^-_F(u)$, respectively. Since $\sum_{u \in V(G)} d^+_F(u) = \sum_{u \in V(G)} d^-_F(u) = |A(F)|$, there exists at least one vertex $u \in V(G)$ such that $d^+_F(u) \geq d^-_F(u)$. So $X \neq \emptyset$.

In this section, we will show some basic properties of $cM_2(G)$ by observation in Lemmas 1 and 2 and introduce two graph operations that will increase $cM_2(G)$ in Lemmas 3 and 4.

Lemma 1. *For any mixed graph F' obtained by orienting some edges in G, we have*

$$cM_2(G) \geq \sum_{\overrightarrow{uv} \in A(F')} (d_{F'}(u)^2 - d_{F'}(v)^2).$$

If the mixed graph $F' = F$, the equality holds.

Lemma 2. *For any mixed graph F' obtained by orienting some edges in G, we have*

$$\begin{aligned} cM_2(G) &\geq \sum_{\overrightarrow{uv} \in A(F')} (d_{F'}(u)^2 - d_{F'}(v)^2) \quad \text{(by Lemma 1)} \\ &= \sum_{v \in V(G)} \Big(- \sum_{\overrightarrow{uv} \in A(F')} d_{F'}(v)^2 + \sum_{\overrightarrow{vw} \in A(F')} d_{F'}(v)^2\Big) \\ &= \sum_{v \in V(G)} (d^+_{F'}(v) - d^-_{F'}(v)) d_{F'}(v)^2. \end{aligned}$$

If the mixed graph $F' = F$, the equality holds.

Lemma 3. *For any $u, v \in X$, if $uv \notin E(G)$, then $cM_2(G + uv) \geq cM_2(G)$. If the equality holds, then $d_F(u) = d_F(v)$, $d^+_F(u) = d^-_F(u)$ and $d^+_F(v) = d^-_F(v)$.*

Proof. Without loss of generality, suppose $d_G(u) \geq d_G(v)$. Add $\overrightarrow{uv}$ to F. Then for any vertex v' in G except u and v, the degree, out-degree, and in-degree of v' in $F + \overrightarrow{uv}$ are the same as in F. Note that since $u, v \in X$, $d^+_F(u) \geq d^-_F(u)$ and $d^+_F(v) \geq d^-_F(v)$. Then, we have

$$\begin{aligned} & cM_2(G + uv) - cM_2(G) \\ & \geq \sum_{v' \in V(G)} (d^+_{F+\overrightarrow{uv}}(v') - d^-_{F+\overrightarrow{uv}}(v')) d_{F+\overrightarrow{uv}}(v')^2 \\ & \quad - \sum_{v' \in V(G)} (d^+_F(v') - d^-_F(v')) d_F(v')^2 \quad \text{(by Lemma 2)} \\ & = (d^+_{F+\overrightarrow{uv}}(u) - d^-_{F+\overrightarrow{uv}}(u)) d_{F+\overrightarrow{uv}}(u)^2 + (d^+_{F+\overrightarrow{uv}}(v) - d^-_{F+\overrightarrow{uv}}(v)) d_{F+\overrightarrow{uv}}(v)^2 \\ & \quad - ((d^+_F(u) - d^-_F(u)) d_F(u)^2 + (d^+_F(v) - d^-_F(v)) d_F(v)^2) \\ & = (d^+_F(u) + 1 - d^-_F(u))(d_F(u) + 1)^2 + (d^+_F(v) - d^-_F(v) - 1)(d_F(v) + 1)^2 \\ & \quad - ((d^+_F(u) - d^-_F(u)) d_F(u)^2 + (d^+_F(v) - d^-_F(v)) d_F(v)^2) \\ & = (d^+_F(u) - d^-_F(u))(2d_F(u) + 1) + (d^+_F(v) - d^-_F(v))(2d_F(v) + 1) \\ & \quad + (d_F(u) + 1)^2 - (d_F(v) + 1)^2 \\ & \geq 0 \;\; \text{(since } d^+_F(u) \geq d^-_F(u),\ d^+_F(v) \geq d^-_F(v) \text{ by } u, v \in X \text{ and } d_G(u) \geq d_G(v)). \end{aligned}$$

If $cM_2(G + uv) = cM_2(G)$, then the second "≥" should be "=", which induces that $d_F(u) = d_F(v)$, $d^+_F(u) = d^-_F(u)$ and $d^+_F(v) = d^-_F(v)$.

Lemma 4. *For any $u, w \in V, v \in Y$, if $\overrightarrow{uv}, \overrightarrow{vw} \in A(F)$, $uw \notin E(G)$, then $cM_2(G - uv - vw + uw) > cM_2(G)$.*

Proof. Notice that $G - uv - vw + uw$ is the underlying graph of the mixed graph $F - \overrightarrow{uv} - \overrightarrow{vw} + \overrightarrow{uw}$, and for any vertex v' in G except v, the degree, out-degree, and in-degree of v' in $F - \overrightarrow{uv} - \overrightarrow{vw} + \overrightarrow{uw}$ are same as in F. Hence, we have

$$\begin{aligned}
& cM_2(G - uv - vw + uw) - cM_2(G) \\
& \geq (d^+_{F-\overrightarrow{uv}-\overrightarrow{vw}+\overrightarrow{uw}}(v) - d^-_{F-\overrightarrow{uv}-\overrightarrow{vw}+\overrightarrow{uw}}(v))d_{F-\overrightarrow{uv}-\overrightarrow{vw}+\overrightarrow{uw}}(v)^2 \\
& \quad - (d^+_F(v) - d^-_F(v))d_F(v)^2 \quad \text{(by Lemma 2)} \\
& = ((d^+_F(v) - 1) - (d^-_F(v) - 1))(d_F(v) - 2)^2 - (d^+_F(v) - d^-_F(v))d_F(v)^2 \\
& = -4(d^+_F(v) - d^-_F(v))(d_F(v) - 1) \\
& > 0 \quad (\text{since } d^+_F(v) < d^-_F(v) \text{ by } v \in Y).
\end{aligned}$$

3. Proofs of Theorems 1 and 2

Proof of Theorem 1: Suppose $G = (V, E)$ is an undirected graph with n vertices and maximum complementary second Zagreb index. Let F be the mixed graph as the last section stated. Then, we will show that G is isomorphic to $K_m \vee \overline{K_{n-m}}$ for some $1 \leq m \leq n - 1$.

Claim 1. *For any $u, v \in X$, if $uv \notin E(G)$, then $d_G(u) = d_G(v)$, and for any $w \in X \setminus \{u, v\}$, $d_G(w) \neq d_G(u)$.*

Proof. By Lemma 3, $cM_2(G + uv) \geq cM_2(G)$. Since G has maximum complementary second Zagreb index, $cM_2(G + uv) = cM_2(G)$. Hence, by Lemma 3, $d_G(u) = d_G(v)$, $d^+_F(u) = d^-_F(u)$ and $d^+_F(v) = d^-_F(v)$.

Suppose to the contrary that there exists $w \in X \setminus \{u, v\}$ such that $d_G(w) = d_G(u)$.

Case 1: If $uw \neq E(G)$, then by Lemma 3, $d^+_F(w) = d^-_F(w)$. Add $\overrightarrow{uv}$ and $\overrightarrow{uw}$ to F. Then, we have

$$\begin{aligned}
& cM_2(G + uv + uw) - cM_2(G) \\
& \geq \sum_{v'=u,v,w} (d^+_{F+\overrightarrow{uv}+\overrightarrow{uw}}(v') - d^-_{F+\overrightarrow{uv}+\overrightarrow{uw}}(v'))d_{F+\overrightarrow{uv}+\overrightarrow{uw}}(v')^2 \\
& \quad - \sum_{v'=u,v,w} (d^+_F(v') - d^-_F(v'))d_F(v')^2 \quad \text{(by Lemma 2)} \\
& = 2(d_F(u) + 2)^2 - (d_F(v) + 1)^2 - (d_F(w) + 1)^2 \\
& \quad (\text{since } d^+_F(u) = d^-_F(u) \text{ ,} d^+_F(v) = d^-_F(v) \text{ and } d^+_F(w) = d^-_F(w)) \\
& > 0,
\end{aligned}$$

contradicting that G has a maximum complementary second Zagreb index.

Case 2: If $uw \in E(G)$, since $d_G(u) = d_G(w)$, $uw \in E(F)$. Consider the mixed graph $F - uw + \overrightarrow{uw} + \overrightarrow{uv}$, whose underlying graph is $G + uv$.

$$
\begin{aligned}
&cM_2(G+uv)-cM_2(G)\\
&\geq \sum_{v'=u,v,w}(d^+_{F-uw+\overrightarrow{uw}+\overrightarrow{uv}}(v')-d^-_{F-uw+\overrightarrow{uw}+\overrightarrow{uv}}(v'))d_{F-uw+\overrightarrow{uw}+\overrightarrow{uv}}(v')^2\\
&\quad-\sum_{v'=u,v,w}(d^+_F(v')-d^-_F(v'))d_F(v')^2 \quad \text{(by Lemma 2)}\\
&\geq 2(d_F(u)+1)^2-(d_F(v)+1)^2+(d^+_F(w)-d^-_F(w)-1)d_F(w)^2\\
&\quad-(d^+_F(w)-d^-_F(w))d_F(w)^2 \quad (\text{since } d^+_F(u)=d^-_F(u) \text{ and } d^+_F(v)=d^-_F(v))\\
&=2(d_F(u)+1)^2-(d_F(v)+1)^2-d_F(w)^2\\
&>0 \quad (\text{since } d_G(u)=d_G(v)=d_G(w)),
\end{aligned}
$$

contradicting that G has a maximum complementary second Zagreb index.

Above all, for any $w \in X$, $d_G(w) \neq d_G(u)$.

Corollary 1. *For any $u \in X$, $d_{G[X]}(u) \geq |X|-2$.*

Proof. Let $u \in X$. Suppose to the contrary that $d_{G[X]}(u) < |X|-2$. Let v be a vertex in X nonadjacent to u. For any $w \in X \setminus \{u,v\}$, since $uv \notin E(G)$, by Claim 1, we have $d_G(w) \neq d_G(u)$; thus we have $uw \in E(G)$ (in fact, suppose to the contrary that $uw \notin E(G)$. Then by Claim 1, we have $d_G(u) = d_G(w)$, contradicting that $d_G(w) \neq d_G(u)$). So, v is the only vertex in X nonadjacent to u, contradicting that $d_{G[X]}(u) < |X|-2$.

Claim 2. *For any $u, v \in Y$, if $uv \in E(G)$, then $uv \notin E(F)$.*

Proof. Suppose to the contrary that $uv \in E(F)$ for some $u, v \in Y$. Note that since $u, v \in Y$, $d^+_F(u) < d^-_F(u)$ and $d^+_F(v) < d^-_F(v)$. Then,

$$
\begin{aligned}
&cM_2(G-uv)-cM_2(G)\\
&\geq (d^+_{F-uv}(u)-d^-_{F-uv}(u))d_{F-uv}(u)^2+(d^+_{F-uv}(v)-d^-_{F-uv}(v))d_{F-uv}(v)^2\\
&\quad-((d^+_F(u)-d^-_F(u))d_F(u)^2+(d^+_F(v)-d^-_F(v))d_F(v)^2) \quad \text{(by Lemma 2)}\\
&=-((d^+_F(u)-d^-_F(u))(2d_F(u)-1)-((d^+_F(v)-d^-_F(v))(2d_F(v)-1)\\
&>0 \quad (\text{since } d^+_F(u)<d^-_F(u) \text{ and } d^+_F(v)<d^-_F(v) \text{ by } u,v\in Y),
\end{aligned}
$$

contradicting that G has a maximum complementary second Zagreb index.

Claim 3. *Suppose $v \in Y$ and $N^-_F(v) \subseteq X$. Then for any $u \in X$, if $uv \in E(G)$, then $\overrightarrow{uv} \in A(F)$.*

Proof. Suppose to the contrary that $uv \in E(F)$ or $\overrightarrow{vu} \in A(F)$ for some $u \in X$.

For any $w \in N^-_F(v)$, that is, $\overrightarrow{wv} \in A(F)$, we can show that $\overrightarrow{wu} \in A(F)$, and thus $d^-_F(u) \geq d^-_F(v)$. In fact, since $\overrightarrow{wv} \in A(F)$, we have $d_G(w) > d_G(v)$; since $uv \in E(F)$ or $\overrightarrow{vu} \in A(F)$, we have $d_G(v) \geq d_G(u)$ and thus $d_G(w) > d_G(u)$. Since $N^-_F(v) \subseteq X$, we have $w \in X$; since $d_G(w) > d_G(u)$, by Claim 1, we have $wu \in E(G)$ and thus $\overrightarrow{wu} \in A(F)$.

Since $u \in X$ and $v \in Y$, we have $d^+_F(u) \geq d^-_F(u)$, and $d^+_F(v) < d^-_F(v)$. Note that $d^-_F(u) \geq d^-_F(v)$. Hence, $d^+_F(u) \geq d^-_F(u) \geq d^-_F(v) > d^+_F(v)$ and thus $d^+_F(u) + d^-_F(u) > d^-_F(v) + d^+_F(v)$.

Case 1: $uv \in E(F)$ (See Figure 1).

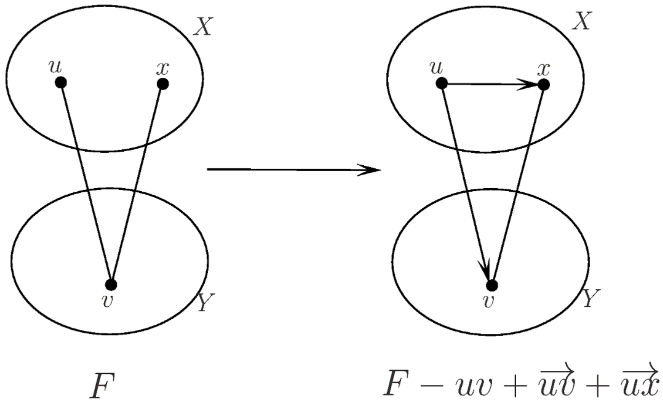

Figure 1. Case 1: $uv \in E(F)$.

Since $uv \in E(F)$, we have $d_F(u) = d_F(v)$, and thus there exists $x \in V(G)$ such that $xv \in E(F)$ and $xu \notin E(F)$. Since $v \in Y$, by Claim 2, we have $x \in X$; since $xu \notin E(F)$, that is, $xu \notin E(G)$, by Claim 1, we have $d_G(x) = d_G(u)$.

$$
\begin{aligned}
& cM_2(G+ux) - cM_2(G) \\
\geq & \sum_{v'=u,x,v} (d^+_{F-uv+\overrightarrow{uv}+\overrightarrow{ux}}(v') - d^-_{F-uv+\overrightarrow{uv}+\overrightarrow{ux}}(v'))d_{F-uv+\overrightarrow{uv}+\overrightarrow{ux}}(v')^2 \\
& - \sum_{v'=u,x,v} (d^+_F(v') - d^-_F(v'))d_F(v')^2 \quad \text{(by Lemma 2)} \\
= & \ 2(d_F(u)+1)^2 - (d_F(x)+1)^2 + (d^+_F(v) - d^-_F(v) - 1)d_F(v)^2 \\
& - (d^+_F(v) - d^-_F(v))d_F(v)^2 \\
& \text{(since } d^+_F(u) = d^-_F(u) \text{ and } d^+_F(x) = d^-_F(x) \text{ by Lemma 3)} \\
= & \ 2(d_F(u)+1)^2 - (d_F(x)+1)^2 - d_F(v)^2 \\
> & \ 0 \quad \text{(since } d_G(u) = d_G(v) = d_G(x)\text{)},
\end{aligned}
$$

contradicting that G has a maximum complementary second Zagreb index.

Case 2: $\overrightarrow{vu} \in A(F)$.

By Case 1, we know that there exists no vertex $w \in X$ such that $wv \in E(F)$; by Claim 2, there exists no vertex $w \in Y$ such that $wv \in E(F)$. Hence, there exists no edge in $E(F)$ incident with v and thus $d_F(v) = d^+_F(v) + d^-_F(v)$. Note that $d^+_F(u) + d^-_F(u) > d^-_F(v) + d^+_F(v)$. Hence, $d_F(u) > d_F(v)$. However, since $\overrightarrow{vu} \in A(F)$, we have $d_F(v) > d_F(u)$, a contradiction.

Claim 4. *$G[Y]$ is empty.*

Proof. Suppose to the contrary that $G[Y]$ is not empty. By Claim 2, $F[Y]$ is a nonempty digraph. Choose a vertex $u \in Y$ such that $d^+_{F[Y]}(u) > 0$ and $d_F(u)$ is maximum. Then, we can show that $N^-_F(u) \subseteq X$. Suppose to the contrary that there exists $w \in Y$ such that $\overrightarrow{wu} \in A(F)$. Then $d_F(w) > d_F(u)$ and $d^+_{F[Y]}(w) > 0$, a contradiction to the choice of u.

Since $N^-_F(u) \subseteq X$, by Claim 3, we have $N^+_F(u) \subseteq Y$. Suppose $N^+_F(u)$ consists of $v_1, v_2, \ldots, v_t$. Denote $E := \{uv_1, uv_2, \ldots, uv_t\}$ and $\overrightarrow{E} := \{\overrightarrow{uv_1}, \overrightarrow{uv_2}, \ldots, \overrightarrow{uv_t}\}$. For any $x \in N^-_F(u)$ and $v_i \in N^+_F(u)$, we can show that $xv_i \in E(G)$. Suppose to the contrary that $xv_i \notin E(G)$. Then by Lemma 4, we have

$cM_2(G + xv_i) > cM_2(G)$, a contradiction. Thus, $xv_i \in E(G)$, that is $\overrightarrow{xv_i} \in A(F)$. Hence, for any $v_i \in N_F^+(u)$, $N_F^-(v_i) \supseteq N_F^-(u) \cup \{u\}$ and we have $d_F^-(v_i) > d_F^-(u)$.

$$\begin{aligned}
&cM_2(G - E) - cM_2(G)\\
&\geq \sum_{v'=u,v_1,\ldots,v_t} (d^+_{F-\overrightarrow{E}}(v') - d^-_{F-\overrightarrow{E}}(v'))d_{F-\overrightarrow{E}}(v')^2\\
&\quad - \sum_{v'=u,v_1,\ldots,v_t} (d_F^+(v') - d_F^-(v'))d_F(v')^2 \quad \text{(by Lemma 2)}\\
&= -d_F^-(u)^3 + \sum_{i=1}^{t}(d_F^+(v_i) - (d_F^-(v_i) - 1))(d_F(v_i) - 1)^2\\
&\quad - (d_F^+(u) - d_F^-(u))d_F(u)^2 - \sum_{i=1}^{t}(d_F^+(v_i) - d_F^-(v_i))d_F(v_i)^2\\
&= -d_F^+(u)^3 + (d_F^-(u) - d_F^+(u))d_F^+(u)d_F^-(u)\\
&\quad + \sum_{i=1}^{t}((d_F(v_i) - 1)^2 + (d_F^-(v_i) - d_F^+(v_i))(2d_F(v_i) - 1))\\
&\quad \text{(since } d_F(u) = d_F^+(u) + d_F^-(u))\\
&> -d_F^+(u)^3 + \sum_{i=1}^{t}(d_F(v_i) - 1)^2 \text{ (since } d_F^-(v_i) > d_F^+(v_i),\ d_F^-(u) > d_F^+(u))\\
&\geq -d_F^+(u)^3 + \sum_{i=1}^{t} d_F^-(u)^2 \quad \text{(since } d_F(v_i) \geq d_F^-(v_i) > d_F^-(u)\text{)}\\
&= -d_F^+(u)^3 + d_F^+(u)d_F^-(u)^2\\
&> 0 \quad \text{(since } d_F^-(u) > d_F^+(u)),
\end{aligned}$$

a contradiction.

Corollary 2. *For any $u \in X$ and $v \in Y$, if $uv \in E(G)$, then $\overrightarrow{uv} \in A(F)$.*

Proof. Let $u \in X$, $v \in Y$ with $uv \in E(G)$. By Claim 4, $N_F^-(v) \subseteq X$; by Claim 3, since $uv \in E(G)$, we have $\overrightarrow{uv} \in A(F)$.

Claim 5. *For any $u, v \in X$, if $d_G(u) \geq d_G(v)$, then, $N_F^+(u) \cap Y \supseteq N_F^+(v) \cap Y$.*

Proof. First, we show that $d_F^-(u) \leq d_F^-(v)$. For any $w \in N^-_{F[X]}(u)$, that is, $w \in X$ and $\overrightarrow{wu} \in A(F)$, we have $d_G(w) > d_G(u)$; since $d_G(u) \geq d_G(v)$, $d_G(w) > d_G(v)$. By Claim 1, $wv \in E(G)$, and thus, $\overrightarrow{wv} \in A(F)$, that is $w \in N^-_{F[X]}(v)$. Hence, $N^-_{F[X]}(u) \subseteq N^-_{F[X]}(v)$. Similarly, $N^+_{F[X]}(u) \supseteq N^+_{F[X]}(v)$. By Corollary 2, $N^-_{F[X]}(u) = N_F^-(u)$ and $N^-_{F[X]}(v) = N_F^-(v)$. Hence, $N_F^-(u) \subseteq N_F^-(v)$, and thus, $d_F^-(u) \leq d_F^-(v)$.

Next, we show that $d_F^+(u) \geq d_F^+(v)$. For any $x \in X$, $d_F^+(x) = |N_F^+(x) \cap Y| + |N^+_{F[X]}(x)|$. Since $|N^+_{F[X]}(u)| \geq |N^+_{F[X]}(v)|$, we only need to prove $|N_F^+(u) \cap Y| \geq |N_F^+(v) \cap Y|$. Note that $|N_F^+(x) \cap Y| = d_F(x) - d_{F[X]}(x)$.

If $d_G(u) > d_G(v)$, since $|X| - 2 \leq d_{G[X]}(u), d_{G[X]}(v) \leq |X| - 1$ by Corollary 1, we have $d_F(u) - d_{F[X]}(u) \geq d_F(v) + 1 - (|X| - 1) \geq d_F(v) - d_{F[X]}(v)$. If $d_G(u) = d_G(v)$, then we can show that $d_{F[X]}(u) = d_{F[X]}(v)$. In fact, suppose to the contrary that $d_{F[X]}(u) = |X| - 2$ and $d_{F[X]}(v) = |X| - 1$ without loss of generality. Let

w be the only vertex in X nonadjacent to u. Since $d_{F[X]}(v) = |X| - 1$, $v \neq w$; by Claim 1, $d_G(v) \neq d_G(u)$, a contradiction.

Finally, we show $N_F^+(u) \cap Y \supseteq N_F^+(v) \cap Y$. Suppose to the contrary that there exists $w \in N_F^+(v) \cap Y \setminus N_F^+(u) \cap Y$. Then,

$$\begin{aligned}
&cM_2(G - vw + uw) - cM_2(G)\\
&\geq \sum_{v'=u,v} (d^+_{F-\overrightarrow{vw}+\overrightarrow{uw}}(v') - d^-_{F-\overrightarrow{vw}+\overrightarrow{uw}}(v'))d_{F-\overrightarrow{vw}+\overrightarrow{uw}}(v')^2\\
&\quad - \sum_{v'=u,v} (d_F^+(v') - d_F^-(v'))d_F(v')^2 \quad \text{(by Lemma 2)}\\
&= (d_F^+(u) + 1 - d_F^-(u))(d_F(u) + 1)^2 + (d_F^+(v) - 1 - d_F^-(v))(d_F(v) - 1)^2\\
&\quad - (d_F^+(u) - d_F^-(u))d_F(u)^2 - (d_F^+(v) - d_F^-(v))d_F(v)^2\\
&= (d_F(u) + 1)^2 - (d_F(v) - 1)^2 + (d_F^+(u) - d_F^-(u))(2d_F(u) + 1)\\
&\quad - (d_F^+(v) - d_F^-(v))(2d_F(v) - 1)\\
&> (d_F^+(u) - d_F^+(v) + d_F^-(v) - d_F^-(u))(2d_F(v) - 1) \quad \text{(since } d_F(u) \geq d_F(v))\\
&\geq 0 \quad \text{(since } d_F^+(u) \geq d_F^+(v) \text{ and } d_F^-(u) \leq d_F^-(v)),
\end{aligned}$$

a contradiction.

Claim 6. *For any $u, v \in X$, $N_F^+(u) \cap Y = N_F^+(v) \cap Y$.*

Proof. Suppose to the contrary that there exist $u_0, v_0 \in X$ such that $N_F^+(u_0) \cap Y \neq N_F^+(v_0) \cap Y$. By Claim 5, suppose that $d_G(u_0) > d_G(v_0)$ and thus $N_F^+(u_0) \cap Y \supsetneq N_F^+(v_0) \cap Y$ without loss of generality. Let $w_0 \in (N_F^+(u_0) \setminus N_F^+(v_0)) \cap Y$.

For any $x \in N_F^-(w_0)$, since $w_0 \in (N_F^+(x) \setminus N_F^+(v_0)) \cap Y$, we have $N_F^+(x) \cap Y \nsubseteq N_F^+(v_0) \cap Y$. By Claim 5, we have $N_F^+(x) \cap Y \supsetneq N_F^+(v_0) \cap Y$ and $d_G(x) > d_G(v_0)$. By Claim 1, $xv_0 \in E(G)$ and thus $\overrightarrow{xv_0} \in A(F)$, that is, $x \in N_F^-(v_0)$. Hence, $N_F^-(w_0) \subseteq N_F^-(v_0)$ and $d_F^-(w_0) \leq d_F^-(v_0)$. Since $v_0 \in X$, we have $d_F^+(v_0) \geq d_F^-(v_0)$ and thus $d_F(v_0) \geq 2d_F^-(w_0)$.

$$\begin{aligned}
&cM_2(G + v_0w_0) - cM_2(G)\\
&\geq \sum_{v'=v_0,w_0} (d^+_{F+\overrightarrow{v_0w_0}}(v') - d^-_{F+\overrightarrow{v_0w_0}}(v'))d_{F+\overrightarrow{v_0w_0}}(v')^2\\
&\quad - \sum_{v'=v_0,w_0} (d_F^+(v') - d_F^-(v'))d_F(v')^2 \quad \text{(by Lemma 2)}\\
&= (d_F^+(v_0) + 1 - d_F^-(v_0))(d_F(v_0) + 1)^2 + (-d_F^-(w_0) - 1)(d_F^-(w_0) + 1)^2\\
&\quad - ((d_F^+(v_0) - d_F^-(v_0))d_F(v_0)^2 + (-d_F^-(w_0)^3))\\
&\quad \text{(since } d_F^+(w_0) = 0 \text{ by Claim 4 and Corollary 2)}\\
&\geq (d_F(v_0) + 1)^2 - (3d_F^-(w_0)^2 + 3d_F^-(w_0) + 1)\\
&\quad \text{(since } d_F^+(v_0) \geq d_F^-(v_0) \text{ by } v_0 \in X)\\
&\geq (2d_F^-(w_0) + 1)^2 - (3d_F^-(w_0)^2 + 3d_F^-(w_0) + 1) \text{ (since } d_F(v_0) \geq 2d_F^-(w_0))\\
&= d_F^-(w_0)^2 + d_F^-(w_0)\\
&> 0,
\end{aligned}$$

a contradiction.

Corollary 3. *For any $u \in X$, $N_F^+(u) \supseteq Y$.*

Proof. For any $v \in Y$, we have $d_F^-(v) > d_F^+(v) \geq 0$; by Claim 4 and Corollary 2, there exists $w \in X$ such that $\overrightarrow{wv} \in A(F)$, that is $v \in N_F^+(w) \cap Y$. By Claim 6, we have $N_F^+(w) \cap Y = N_F^+(u) \cap Y$ and thus $v \in N_F^+(u) \cap Y$. Hence, $Y \subseteq N_F^+(u) \cap Y$, that is $Y \subseteq N_F^+(u)$.

By Corollary 1, denote $X_1 := \{u \in X : d_{G[X]}(u) = |X| - 1\}$ and $X_2 := \{u \in X : d_{G[X]}(u) = |X| - 2\}$. By Corollary 3, we have $d_G(u) = |X| + |Y| - 1$ for $u \in X_1$ and $d_G(u) = |X| + |Y| - 2$ for $u \in X_2$. Next, we will show that $X_2 = \emptyset$ and thus G is isomorphic to $K_{|X|} \vee \overline{K_{n-|X|}}$, completing the proof.

Suppose to the contrary that $X_2 \neq \emptyset$. Let $u \in X_2$, that is, $d_{G[X]}(u) = |X| - 2$. Let $v \in X$ be the only nonadjacent vertex to u in $G[X]$. Then $v \in X_2$ and by Corollary 1, for any $w \in X \setminus \{u, v\}$, we have $d_G(w) \neq d_G(u)$ and thus $w \in X_1$. Hence, $X_2 = \{u, v\}$ and $G[X] + uv$ is a complete graph. By Corollary 3, $N_F^+(u) = Y$. Since $u, v \in X$ and $uv \notin E(G)$, by Lemma 3, we have $d_F^-(u) = d_F^+(u)$, that is, $|X_1| = |Y|$. So $|X| = |Y| + 2$. Note that $G + uv$ is isomorphic to $K_{|X|} \vee \overline{K_{|Y|}}$, and

$$\begin{aligned}
&cM_2(K_{|X|} \vee \overline{K_{|Y|}}) - cM_2(G) \\
&= cM_2(G + uv) - cM_2(G) \\
&\geq cM_2(F + uv) - cM_2(F) \\
&= \sum_{v'=u,v} (d_{F+uv}^+(v') - d_{F+uv}^-(v'))(d_F(v'))^2 - \sum_{v'=u,v} (d_F^+(v') - d_F^-(v'))(d_F(v'))^2 \\
&= 0.
\end{aligned}$$

Since $|X| = |Y| + 2$, we have $cM_2(K_{|Y|} \vee \overline{K_{|X|}}) = |X||Y|((n-1)^2 - |Y|^2) > cM_2(K_{|X|} \vee \overline{K_{|Y|}}) = |X||Y|((n-1)^2 - |X|^2)$, a contradiction.

Proof of Theorem 2: Consider

$$\begin{aligned}
cM_2(K_m \vee \overline{K_{n-m}}) &= m(n-m)((n-1)^2 - m^2) \\
&= n^4((\frac{m}{n})^4 - (\frac{m}{n})^3 - (\frac{n-1}{n})^2(\frac{m}{n})^2 + (\frac{n-1}{n})^2\frac{m}{n}).
\end{aligned}$$

Suppose to the contrary that $m_n \geq \frac{n}{2}$. If $m_n > \frac{n}{2}$, then $cM_2(K_{n-m_n} \vee \overline{K_{m_n}}) - cM_2(K_{m_n} \vee \overline{K_{n-m_n}}) = m_n(n-m_n)(m_n^2 - (n-m_n)^2) > 0$, a contradiction; if $m_n = \frac{n}{2}$, then $cM_2(K_{\frac{n}{2}-1} \vee \overline{K_{\frac{n}{2}+1}}) - cM_2(K_{\frac{n}{2}} \vee \overline{K_{\frac{n}{2}}}) = \frac{1}{4}n(n-2)^2 > 0$, a contradiction. This proves that $\frac{m_n}{n} < \frac{1}{2}$.

Denote $f_n(x) := x^4 - x^3 - (\frac{n-1}{n})^2 x^2 + (\frac{n-1}{n})^2 x$, where $x \in [0, 1]$. Then $cM_2(K_m \vee \overline{K_{n-m}}) = n^4 f_n(\frac{m}{n})$. Recall that m_n is such that $cM_2(K_{m_n} \vee \overline{K_{n-m_n}})$ reaches the maximum complementary second Zagreb index among all graphs of order n. So $f_n(\frac{m_n}{n})$ reaches the maximum of $f_n(x)$, where $x \in \{\frac{1}{n}, \frac{2}{n}, \ldots, \frac{n-1}{n}\}$.

Note that $f_n'(x) = 4x^3 - 3x^2 - 2(\frac{n-1}{n})^2 x + (\frac{n-1}{n})^2$, $f_n'(-1) < 0$, $f_n'(0) > 0$, $f_n'(\frac{1}{2}) < 0$, and $f_n'(1) > 0$. According to the Intermediate Value Theorem for continuous functions, there exists $r_1^n \in (-1, 0)$, $r_2^n \in (0, \frac{1}{2})$, $r_3^n \in (\frac{1}{2}, 0)$ such that $f_n'(r_1^n) = f_n'(r_2^n) = f_n'(r_3^n) = 0$, $f_n'(x) < 0$ when $x \in (-\infty, r_1^n) \cup (r_2^n, r_3^n)$, and $f_n'(x) > 0$ when $x \in (r_1^n, r_2^n) \cup (r_3^n, +\infty)$. So, $f_n(x)$ is monotonically increasing on $[0, r_2^n]$, monotonically decreasing on $[r_2^n, r_3^n]$ and monotonically increasing on $[r_3^n, 1]$. Hence, $f_n(r_2^n)(> f_n(1) = 0)$ reaches the maximum of $f_n(x)$, where $x \in [0, 1]$.

Note that r_2^n is between two numbers of $\{\frac{1}{n}, \frac{2}{n}, \ldots, \frac{n-1}{n}\}$, one of which, by the monotonicity of $f_n(x)$, must be $\frac{m_n}{n}$. So

$$|\frac{m_n}{n} - r_2^n| < \frac{1}{n}. \tag{3.1}$$

Denote $g(x) := 4x^3 - 3x^2 - 2x + 1$. Note that $r_1 = \frac{-\sqrt{17}-1}{8}$, $r_2 = \frac{\sqrt{17}-1}{8}$, $r_3 = 1$ are the roots of $g(x) = 0$. Let $\mathbf{C}$ be the field of complex numbers. A classical result states that the roots of a polynomial with coefficients in $\mathbf{C}$ are continuous functions of the coefficients of the polynomial. Further details and a simple new proof are available in [13]. Since the coefficients of $f_n'(x)$ tend to the coefficients of $g(x)$ when $n \to \infty$, we have $\lim_{n\to\infty} r_2^n = r_2 = \dfrac{\sqrt{17}-1}{8}$. By (3.1), we have $\lim_{n\to\infty} \dfrac{m_n}{n} = \dfrac{\sqrt{17}-1}{8}$.

4. Concluding remarks

In this work, we have found the graph having a maximum complementary second Zagreb index among all graphs of order n. Following a helpful suggestion of the reviewer, it would be worthwhile to mention the definition of "cM_2-maximal". A graph G is cM_2-maximal if for any $e \notin E(G)$, $cM_2(G) > cM_2(G + e)$. Obviously, the graph with the maximum complementary second Zagreb index is, of course, cM_2-maximal. Moreover, there are numerous other cM_2-maximal graphs such that it's more complicated to determine all cM_2-maximal graphs. For example, we show a class of cM_2-maximal graphs with only two degrees.

Let m, n, k be positive integers with $k + 1 < \min\{n - m, m + 1\}$, let H_1 be a complete graph of order m and H_2 be a regular graph of degree k and order $n - m$. Let $G := H_1 \vee H_2$. Then, we can show that G is cM_2-maximal. Since $k < n - m - 1$, H_2 is not a complete graph. Let $u, v \in V(H_2)$ be any two nonadjacent vertices. It's straightforward to calculate

$$cM_2(G) = m(n - m)((n - 1)^2 - (k + m)^2),$$

$$\begin{aligned} cM_2(G + uv) = {} & m(n - m - 2)((n - 1)^2 - (k + m)^2) \\ & + 2m((n - 1)^2 - (k + m + 1)^2) + 2k((k + m + 1)^2 - (k + m)^2). \end{aligned}$$

Then since $m > k$, we have

$$cM_2(G) - cM_2(G + uv) = 2(m - k)((k + m + 1)^2 - (k + m)^2) > 0.$$

Hence, G is cM_2-maximal.

In a similar way, we can construct many other cM_2-maximal graphs, such as graphs with only three degrees, four degrees, and so on. Hence, determining all cM_2-maximal graphs appears to be an interesting and challenging research topic.

Use of Generative-AI tools declaration

The author declares he has not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The author declares that no conflicts of interest.

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