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Graphs with Maximum Generalized Complementary Second Zagreb Index

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Abstract

In this paper, we confirm a conjecture by Furtula and Oz regarding graphs that maximize the second complementary Zagreb index. We demonstrate that this conjecture holds for a broader class of indices, each of which is parameter-dependent, and which we will refer to as the generalized complementary second Zagreb index. It is shown that all indices in this class are maximized by complete split graphs. Additionally, we analyze the behavior of the clique order in optimal graphs. For the case of the second complementary Zagreb index, we provide an explicit expression, thereby confirming the value conjectured by Furtula and Oz.

1 Introduction

It happens with alarming regularity in mathematical chemistry that different researchers or research teams introduce the same, or essentially equivalent, concepts under different names. A nice example is provided in a

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recent article by Furtula and Oz [4], concerned with the newest incarnation of the index they named the *second complementary Zagreb index*, but also known as the *nano-Zagreb index* [6], the *F-minus index* [7], and the *first Sombor index* [5, 9]. As the cited journals form a rather eclectic collection, it is quite possible that the list of alternative names is not exhaustive.

The second complementary Zagreb index, as formulated by Furtula and Oz, fits nicely into the class of irregularity measures, being the most natural generalization of its archetypal member, the Albertson irregularity index [3]. Like any valid irregularity measure, it attains its minimum value of zero on all regular graphs. The problem of identifying the maximizing graphs, however, is more complex. The cases for trees and unicyclic graphs were resolved in prior studies [10] and [8], respectively, but the general case remained unresolved. Furtula and Oz conjectured that the maximizing graphs must belong to the class of complete split graphs, i.e. graphs consisting of a clique and an empty graph, with edges connecting every vertex in the clique to every vertex in the empty part. Additionally, they provided an estimate for the optimal number of vertices in the clique, based on the total number of vertices in the graph.

In this paper, we first extend the complementary second Zagreb index by introducing its generalized version that encompasses a class of indices depending on a free positive integer parameter. This version is referred to as the generalized complementary second Zagreb index, which yields the complementary second Zagreb index when the parameter is fixed to 2. The necessary concepts and definitions are introduced in Section 2. In Section 3, we show that all indices in this class are maximized by complete split graphs, thereby confirming the conjecture made by Furtula and Oz. Furthermore, in Section 4, we analyze the behavior of the clique order as a function of the parameter. For the case where the parameter is 2, we provide an explicit expression, further confirming the conjectured value obtained by Furtula and Oz. In the final section, we summarize our results and suggest potential directions for future research.

2 Definitions and preliminaries

All graphs considered in this paper are finite, simple, and connected. We assume the reader is familiar with basic notions of the graph theory. We denote the vertex set and the edge set of a graph G by $V(G)$ and $E(G)$, respectively. For a vertex $v \in V(G)$, its *degree* $d_G(v)$ is the number of its neighbors in G. We denote the set of neighbors of a v by $N_G(v)$. Graphs in which all vertices have the same degree are called *regular*. The largest and the smallest degree of a vertex in a graph G we denote by $\Delta(G)$ and $\delta(G)$, respectively. When the graph G is clear from the context, we omit the (G) part (G-subscript). A vertex of degree $|V(G)| - 1$ in G is referred to as a *universal vertex*, while a *pendent vertex* is a vertex of degree 1 in G.

An irregularity measure is any graph invariant $I(G)$ which is equal to zero for all regular graphs on a given number of vertices and nonnegative for non-regular graphs. Naturally, an irregularity measure should achieve its maximum value(s) on graphs which are, in some sense, the farthest from being regular. Different irregularity measures accomplish this in various ways, each capturing and quantifying distinct aspects of non-regularity. Most of these measures are sensitive to local connectivity patterns, and there is no consensus on which one is "the best."

The *Albertson irregularity* of a graph G is defined as the sum of the edge contributions, where each contribution is the absolute value of the difference in degrees of the two vertices incident to that edge. Formally, it is given by

$$irr(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|,$$

where $|d_G(u) - d_G(v)|$ is referred to as the *imbalance* of the edge uv. In other words, the imbalance of an edge is the absolute difference between the degrees of its two end-vertices.

There are several ways to generalize the Albertson irregularity. One of the most straightforward approaches is to raise the edge contributions to a (not necessarily integer) power. Another natural generalization involves raising the vertex degrees to the same power and then considering the absolute value of their difference. The simplest case of this approach occurs when the power is set to two, which yields the second complementary Zagreb index, as defined by Furtula and Oz:

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

It is important to note that Furtula and Oz did not derive this invariant simply by squaring the degrees. Instead, $cM_2(G)$ naturally emerged in their paper as a result of geometric considerations in a plane parameterized by vertex degrees. Their definition avoids the use of absolute values by specifying that, for unequal degrees, the smaller degree is always subtracted from the larger one. Clearly, their definition is equivalent to the one presented in this paper.

There is no reason, however, to stop at the second power. For any given nonnegative integer l, one can define a *generalized complementary second Zagreb index* of a graph G as

$$cM_l(G) = \sum_{uv \in E(G)} \left| d_G^l(u) - d_G^l(v) \right| .$$

By setting $l = 1$ and $l = 2$, it is immediately clear that this new invariant generalizes both the Albertson irregularity and the second complementary Zagreb index of Furtula and Oz, respectively.

In their paper [4], Furtula and Oz focused more on the potential applications of the second complementary Zagreb index than on its mathematical properties. However, they did investigate the graphs that maximize this index for a given number of vertices. After conducting an exhaustive search on small graphs, they proposed the following conjecture regarding the structure and size of the maximizing graphs.

Conjecture 1. *[4]*
Vertices in the connected graph with the maximal complementary second Zagreb index are partitioned into two groups. Let's label the number of vertices in the first group with k, which is always smaller than $\lceil n/2 \rceil$. These vertices form a k-complete subgraph. Each of the other $n - k$ vertices in

this connected graph is connected to all vertices of the k-complete subgraph, but they are not mutually interconnected.

The graphs described in the conjecture are known as complete split graphs. A graph G on n vertices is a *complete split graph* $CS_{k,n-k}$ if k of its vertices induce a clique, i.e., the complete subgraph K_k, the remaining $n-k$ vertices induce the empty subgraph $\overline{K}_{n-k}$, and each vertex of the clique is connected by an edge to each vertex of the empty subgraph. We can write $CS_{k,n-k} = K_k + \overline{K}_{n-k}$, where $+$ denotes the join of two graphs. (For two graphs G and H on disjoint vertex sets, their *join* is obtained by keeping all edges of G and of H and by adding an edge between each vertex of G and each vertex of H.)

Conjecture 1 can now be restated more succinctly as follows: *Any graph that maximizes the complementary second Zagreb index among all graphs on n vertices is a complete split graph $CS_{k,n-k}$ with k not exceeding $\lceil n/2 \rceil$.*

In the next section, we prove that for each $l \geq 1$, the generalized complementary second Zagreb index cM_l is maximized by complete split graphs, thereby confirming Conjecture 1 and reaffirming previously known results regarding the Albertson irregularity.

3 The structure of maximizing graphs

In this section, we examine connected simple graphs on $n \geq 5$ vertices and identify those that maximize cM_l for a given value of l. We begin by demonstrating that the vertices with the largest degree in a maximizing graph induce a complete subgraph.

Lemma 1. *Let G be a graph maximizing $cM_l(G)$ over all connected graphs on n vertices. Then its vertices of degree Δ induce a complete subgraph.*

Proof. Suppose, for the sake of contradiction, that there are vertices u and v in G, both of degree Δ, that are not connected by an edge. Adding the edge uv to G results in a graph $G' = G + uv$, in which the contributions to $cM_l(G)$ of all edges incident with either u or v are strictly greater than their respective contributions in G while the contributions of all other edges remain unchanged. Therefore, $cM_l(G') > cM_l(G)$, which contradicts the assumption that G maximizes $cM_l(G)$. ■

Next, we demonstrate that the vertices of minimum degree in G induce an empty subgraph, meaning that no two of these vertices are adjacent in G.

Lemma 2. *Let G be a graph maximizing $cM_l(G)$ over all connected graphs on n vertices. Then its vertices of degree δ induce an empty subgraph.*

Proof. Suppose, for the sake of contradiction, that there are vertices u and v in G, both of degree δ, that are connected by an edge. Removing this edge from G increases the contributions to $cM_l(G)$ of all edges incident to either u or v, while leaving the contributions of all other edges unchanged. As a result, we obtain a new graph $G' = G - uv$ with the same number of vertices n, and $cM_l(G') > cM_l(G)$, which contradicts the assumption that G maximizes $cM_l(G)$. ■

The next two lemmas show that a maximizing graph must contain universal vertices.

Lemma 3. *Let G be a connected graph with a vertex v of maximum degree Δ. Let u and w be vertices of G such that u is a pendent vertex, $uw \in E(G)$ and $vw \notin E(G)$, $v \neq w$. Then*

$$cM_l(G) < cM_l(G - uw + vw + uv). \tag{1}$$

Proof. Let $N_G(v) = \{x_1, x_2, \ldots, x_\Delta\}$ and let $G' := G - uw + vw + uv$. We denote $\mathrm{D}(G', G) := cM_l(G') - cM_l(G)$. It follows that

$$\begin{aligned}
\mathrm{D}(G', G) = & \sum_{yz \in E(G')} |d^l_{G'}(y) - d^l_{G'}(z)| - \sum_{yz \in E(G)} |d^l_G(y) - d^l_G(z)| \\
&= \sum_{i=1}^{\Delta} [(\Delta+2)^l - d^l_G(x_i)] + (\Delta+2)^l - d^l_G(w) \\
&\quad + (\Delta+2)^l - 1 - \sum_{i=1}^{\Delta} [\Delta^l - d^l_G(x_i)] - (d^l_G(w) - 1)
\end{aligned}$$

$$= \sum_{i=1}^{\Delta}[(\Delta+2)^l - \Delta^l] + 2[(\Delta+2)^l - d_G^l(w)] > 0. \qquad \blacksquare$$

Lemma 4. *Let G be a connected graph with a vertex v of maximum degree Δ. Let u and w be vertices of G such that $d_G(u) \geq 2$, $uw \in E(G)$ and $vw \notin E(G)$, $v \neq w$. Then*

$$cM_l(G) < cM_l(G - uw + vw). \tag{2}$$

Proof. Let $N_G(v) = \{x_1, x_2, \ldots, x_\Delta\}$ and $N_G(u) = \{w, y_1, y_2, \ldots, y_t\}$, $t \geq 1$. Then $d_G(u) = t+1$, which yields $t < \Delta$. We denote $G' := G - uw + vw$. We consider two cases.

Case 1. $uv \notin E(G)$. It follows that

$$\begin{aligned}
\mathrm{D}(G', G) &= \sum_{yz \in E(G')} |d_{G'}^l(y) - d_{G'}^l(z)| - \sum_{yz \in E(G)} |d_G^l(y) - d_G^l(z)| \\
&= \sum_{i=1}^{\Delta}[(\Delta+1)^l - d_G^l(x_i)] + \sum_{i=1}^{t} |t^l - d_G^l(y_i)| \\
&\quad + (\Delta+1)^l - d_G^l(w) - \sum_{i=1}^{\Delta}[\Delta^l - d_G^l(x_i)] \\
&\quad - \sum_{i=1}^{t} |(t+1)^l - d_G^l(y_i)| - |(t+1)^l - d_G^l(w)| \\
&\geq \Delta[(\Delta+1)^l - \Delta^l] - t[(t+1)^l - t^l] \\
&\quad + \min\{(\Delta+1)^l - (t+1)^l, (\Delta+1)^l + (t+1)^l - 2d_G^l(w)\} \\
&= \min\{a, b\},
\end{aligned}$$

where

$$\begin{aligned}
a &= (\Delta+1)^{l+1} - (t+1)^{l+1} - (\Delta^{l+1} - t^{l+1}), \\
b &= (\Delta+1)^{l+1} - (t+1)^l(t-1) - (\Delta^{l+1} - t^{l+1}) - 2d_G^l(w).
\end{aligned}$$

We can immediately conclude that $a > 0$. Let us prove that $b > 0$. By using the formula $x^l - y^l = (x-y)\sum_{i=0}^{l-1} x^i y^{l-1-i}$, we obtain

$$
\begin{aligned}
b &= (\Delta+1)^{l+1} - \Delta^{l+1} - (t+1)^l(t-1) + t^{l+1} - 2d_G^l(w) \\
&= \sum_{i=0}^{l}(\Delta+1)^i\Delta^{l-i} - (t-1)\left[(t+1)^l - t^l\right] + t^l - 2d_G^l(w) \\
&= \sum_{i=0}^{l}(\Delta+1)^i\Delta^{l-i} - (t-1)\sum_{i=0}^{l-1}(t+1)^i t^{l-1-i} + t^l - 2d_G^l(w) \\
&= \Delta^l + (\Delta+1)\Delta^{l-1} + (\Delta+1)^l + \sum_{i=2}^{l-1}(\Delta+1)^i\Delta^{l-i} - (t-1)t^{l-1} \\
&\quad - (t-1)(t+1)t^{l-2} - (t-1)\sum_{i=2}^{l-1}(t+1)^i t^{l-1-i} + t^l - 2d_G^l(w) \\
&= 2(\Delta^l - d_G^l(w)) + [(\Delta+1)^l - t^l] + \Delta^{l-1} + t^{l-2}(t+1) \\
&\quad + \sum_{i=2}^{l-1}[(\Delta+1)^i\Delta^{l-i} - (t+1)^i(t^{l-i} - t^{l-1-i})] > 0.
\end{aligned}
$$

Case 2. $uv \in E(G)$. Then u is one of the vertices $x_1, x_2, \ldots, x_\Delta$ and v is one of the vertices $y_1, y_2, \ldots, y_t$. Without loss of generality, we assume $u = x_\Delta$ and $v = y_t$. Then

$$
\begin{aligned}
\mathrm{D}(G', G) &= \sum_{yz \in E(G')} |d_{G'}^l(y) - d_{G'}^l(z)| - \sum_{yz \in E(G)} |d_G^l(y) - d_G^l(z)| \\
&= \sum_{i=1}^{\Delta-1}[(\Delta+1)^l - d_G^l(x_i)] + \sum_{i=1}^{t-1}|t^l - d_G^l(y_i)| + (\Delta+1)^l - d_G^l(w) \\
&\quad + (\Delta+1)^l - t^l - \sum_{i=1}^{\Delta-1}[\Delta^l - d_G^l(x_i)] - \sum_{i=1}^{t-1}|(t+1)^l - d_G^l(y_i)| \\
&\quad - |(t+1)^l - d_G^l(w)| - [\Delta^l - (t+1)^l] \\
&\geq (\Delta-1)[(\Delta+1)^l - \Delta^l] + (\Delta+1)^l - \Delta^l \\
&\quad + (t+1)^l - t^l - (t-1)[(t+1)^l - t^l] \\
&\quad + \min\{(\Delta+1)^l - (t+1)^l, (\Delta+1)^l + (t+1)^l - 2d_G^l(w)\} \\
&= \min\{a, b\},
\end{aligned}
$$

where

$$a = (\Delta+1)^{l+1} - \Delta^{l+1} - (t-1)\left[(t+1)^l - t^l\right] - t^l,$$
$$b = (\Delta+1)^{l+1} - \Delta^{l+1} - (t-1)\left[(t+1)^l - t^l\right] + 2(t+1)^l - t^l - 2d_G^l(w).$$

Let us prove that $a > 0$ and $b > 0$. We have

$$\begin{aligned} a &= (\Delta+1)^{l+1} - \Delta^{l+1} - (t-1)\left[(t+1)^l - t^l\right] - t^l \\ &= \sum_{i=0}^{l} (\Delta+1)^i \Delta^{l-i} - (t-1)\sum_{i=0}^{l-1}(t+1)^i t^{l-1-i} - t^l \\ &= \left[(\Delta+1)^l - t^l\right] + \sum_{i=0}^{l-1}\left[(\Delta+1)^i\Delta^{l-i} - (t+1)^i(t^{l-i} - t^{l-1-i})\right] > 0. \end{aligned}$$

Furthermore,

$$\begin{aligned} b &= (\Delta+1)^{l+1} - \Delta^{l+1} - (t-1)\left[(t+1)^l - t^l\right] + 2(t+1)^l - t^l - 2d_G^l(w) \\ &= \sum_{i=0}^{l}(\Delta+1)^i\Delta^{l-i} - (t-2)\sum_{i=0}^{l-1}(t+1)^i t^{l-1-i} + (t+1)^l - 2d_G^l(w) \\ &= \left[(\Delta+1)^l + \Delta^l - 2d_G^l(w)\right] + \left[(t+1)^l - t^l + 2t^{l-1}\right] \\ &\quad + \sum_{i=1}^{l-1}\left[(\Delta+1)^i\Delta^{l-i} - (t+1)^i(t^{l-i} - 2t^{l-1-i})\right] > 0. \end{aligned}$$ ■

Note that the transformation of G in Lemma 4 preserves the number of edges in G, whereas the transformation in Lemma 3 increases it.

We can now show that Δ must be equal to $n-1$, i.e., that each vertex of degree Δ must be adjacent to all other vertices.

Corollary 1. *Let G be an n-vertex connected graph which maximizes the generalized complementary second Zagreb index. Then the maximum degree of G is $n-1$.*

Proof. Let v be a vertex of maximum degree in G, and suppose that $d_G(v) < n-1$. Then, there exists a vertex w in G such that $vw \notin E(G)$. Since G is connected, there must be a vertex u in G such that $uw \in E(G)$. If $d_G(u) = 1$, then by Lemma 3 we obtain $cM_l(G) < cM_l(G - uw + vw + uv)$, contradicting the maximality of G. If $d_G(u) \geq 2$, then by Lemma 4 we get $cM_l(G) < cM_l(G - uw + vw)$, again leading to a contradiction. Thus, the assumption is false. ■

The above results indicate that if a graph G maximizes the generalized complementary second Zagreb index, then $\mathrm{diam}(G) = 2$, the vertices with the maximum degree Δ induce a clique in G, and the vertices of the minimum degree induce an empty subgraph. It remains to show that there are no vertices of degrees different from Δ and δ.

Theorem 1. *Let G be a connected n-vertex graph which maximizes the generalized complementary second Zagreb index. Then G is a complete split graph.*

Proof. For an arbitrary graph H we have

$$cM_l(H) = \sum_{\substack{uv\in E(H)\\ d(u)\geq d(v)}} (d^l(u) - d^l(v)) = \sum_{\substack{uv\in E(H)\\ d(u)>d(v)}} (d^l(u) - d^l(v))$$

$$= \sum_{\substack{uv\in E(H)\\ d(u)>d(v)}} (d(u) - d(v)) \sum_{i=0}^{l-1} d^i(u) d^{l-1-i}(v).$$

Let $1 \leq m_1 \leq m$ be the number of edges $u_i v_i$ in H for which $d(u_i) > d(v_i)$, $i = 1, \ldots, m_1$. We define vectors $\vec{x} := [d(u_1) - d(v_1), \ldots, d(u_{m_1}) - d(v_{m_1})]^\tau$ and $\vec{y} := \left[\sum_{i=0}^{l-1} d^i(u_1) d^{l-1-i}(v_1), \ldots, \sum_{i=0}^{l-1} d^i(u_{m_1}) d^{l-1-i}(v_{m_1})\right]^\tau$. The inner product of these vectors is equal to $cM_l(H)$. By applying the Cauchy-Schwarz inequality to them, we obtain

$$cM_l(H) = \sum_{j=1}^{m_1} \left[(d(u_j) - d(v_j)) \sum_{i=0}^{l-1} d^i(u_j) d^{l-1-i}(v_j)\right]$$

$$\leq \sqrt{\sum_{j=1}^{m_1} (d(u_j) - d(v_j))^2} \cdot \sqrt{\sum_{j=1}^{m_1} \left(\sum_{i=0}^{l-1} d^i(u_j) d^{l-1-i}(v_j)\right)^2}. \quad (3)$$

Equality in (3) holds if and only if $\vec{x}$ and $\vec{y}$ are linearly dependent, which in our case means there exists a scalar $\lambda \in \mathbb{Q}$ with $\lambda > 1$ such that $\vec{y} = \lambda \vec{x}$, i.e. the following equalities hold:

$$\begin{aligned}\sum_{i=0}^{l-1} d^i(u_1)d^{l-1-i}(v_1) &= \lambda(d(u_1)-d(v_1)),\\ \sum_{i=0}^{l-1} d^i(u_2)d^{l-1-i}(v_2) &= \lambda(d(u_2)-d(v_2)),\\ &\vdots\\ \sum_{i=0}^{l-1} d^i(u_{m_1})d^{l-1-i}(v_{m_1}) &= \lambda(d(u_{m_1})-d(v_{m_1})).\end{aligned} \tag{4}$$

Denote by G the graph for which equality in (3) holds. Let v be a vertex of maximum degree Δ in G and let $w_1, \ldots, w_p$ be its neighbors, where each w_k satisfies $d(w_k) < \Delta$, for $k = 1, \ldots, p$. Then $1 \leq p \leq \Delta$. We consider equalities (4) for edges vw_k and obtain

$$\begin{aligned}\sum_{i=0}^{l-1} \Delta^i d^{l-1-i}(w_1) &= \lambda(\Delta - d(w_1))\\ \sum_{i=0}^{l-1} \Delta^i d^{l-1-i}(w_2) &= \lambda(\Delta - d(w_2))\\ &\vdots\\ \sum_{i=0}^{l-1} \Delta^i d^{l-1-i}(w_p) &= \lambda(\Delta - d(w_p)),\end{aligned}$$

from which it follows

$$\lambda d(w_k) + \sum_{i=0}^{l-1} \Delta^i d^{l-1-i}(w_k) = \lambda\Delta - \Delta^{l-1}, \quad k = 1, \ldots, p.$$

Since λ and Δ are fixed positive integers, the above expression yields

$$\lambda d(w_{k_1}) + \sum_{i=0}^{l-1} \Delta^i d^{l-1-i}(w_{k_1}) = \lambda d(w_{k_2}) + \sum_{i=0}^{l-1} \Delta^i d^{l-1-i}(w_{k_2}), \qquad (5)$$

for all $k_1, k_2 = 1, \ldots, p$, $k_1 \neq k_2$. Note that (5) holds if and only if $d(w_{k_1}) = d(w_{k_2})$. We conclude that vertices w_k have the same degree. From Corollary 1, we know that $\Delta = n - 1$. Therefore, all neighbors of v, except those of degree Δ, share the same degree. Consequently, we have $d(w_k) = \delta$ for $k = 1, \ldots, p$. Since v was chosen arbitrarily, by applying Lemma 2, we conclude that G is a complete split graph, where the independent set (the subset of vertices of G such that no two of its vertices are adjacent to each other), has cardinality p. For such G we calculate the generalized complementary second Zagreb index and get

$$\begin{aligned} cM_l(G) &= \sqrt{\sum_{j=1}^{m_1} (\Delta - \delta)^2} \cdot \sqrt{\sum_{j=1}^{m_1} \left(\sum_{i=0}^{l-1} \Delta^i \delta^{l-1-i} \right)^2} \\ &= m_1(\Delta^l - \delta^l) \\ &= \sum_{uv \in E(G)} \left[(n-1)^l - \delta^l \right]. \qquad (6) \end{aligned}$$

■

Hence, we have proved that maximizing graphs for a generalized complementary second Zagreb index must be complete split graphs $CS_{k,n-k}$. By taking $l = 2$, our result confirms the main (structural) part of Conjecture 1. The remaining part, concerning the optimal order k of the clique for a given n, will follow from more general results in our next section.

The appearance of split graphs as the maximizers of an irregularity measure is not surprising. They have been already confirmed as the maximizers of the Albertson irregularity [1] and of a related measure called the σ irregularity [2].

4 Optimizing the clique order

In this section we consider the optimal k, i.e., the optimal order of the clique K_k in complete split graph(s) maximizing cM_l for given values of l and n. We start by showing that in all cases k cannot be greater than $\lfloor n/2 \rfloor$.

Lemma 5. *A complete split graph $CS_{k,n-k}$ cannot maximize $cM_l(G)$ over all connected graphs on n vertices for $k > \lfloor n/2 \rfloor$.*

Proof. Let $CS_{k,n-k}$ be a maximizing graph for $cM_l(G)$ and let $k > \lfloor n/2 \rfloor$. Take the graph G' obtained by switching the roles of k and $n-k$ in $CS_{k,n-k} = K_k + \overline{K}_{n-k}$, i.e., $G' = K_{n-k} + \overline{K}_k$, and compute the difference $cM_l(G') - cM_l(G)$.

$$cM_l(G') - cM_l(G) = k(n-k)\left[k^l - (n-k)^l\right] > 0,$$

a contradiction. ■

This settles the remaining part of Conjecture 1.

For $l = 1$, i.e., for Albertson irregularity, the exact value of the optimal k is known. According to Theorem 2.2 of [1], the optimal k is either $\lfloor n/3 \rfloor$, or $\lceil n/3 \rceil$, with the latter case occurring when n divided by 3 gives the remainder 2. Therefore, the next step is to determine the exact value(s) of the optimal k for given n and $l \geq 2$. We begin by considering the case $l = 2$.

The following theorem provides a complete characterization of the graphs that maximize the complementary second Zagreb index. In particular, it determines the optimal number of universal vertices in a graph G, as described in Theorem 1.

Theorem 2. *Let $n \geq 5$ and let G be a connected graph on n vertices maximizing the complementary second Zagreb index among all such graphs.* *(i) If $17n^2 - 28n + 4$ is not a complete square, then G is the complete split graph $CS_{k^*,n-k^*}$, where k^* is the number of universal vertices given by the formula*

$$k^* = \left\lfloor \frac{1}{8}\left[\sqrt{17n^2 - 28n + 4} - (n-6)\right]\right\rfloor, \tag{7}$$

and G is the only such graph;
(ii) If $17n^2-28n+4=s^2$ for some nonnegative integer s and if s and $n-6$ give the same remainder when divided by 8, then G is either $CS_{k^*,n-k^*}$ or $CS_{k^*+1,n-k^*-1}$. If s is not congruent to $n-6$ modulo 8, then G is $CS_{k^*,n-k^*}$.

Proof. Let $n \geq 5$ and let G be a complete split graph with k universal vertices. Then $\Delta(G)=n-1$, $\delta(G)=k$ and $E(G)=k(n-k)$. Inserting this into expression (6) of Theorem 1 and taking $l=2$ we get

$$cM_2(G)=k(n-k)[(n-1)^2-k^2]. \tag{8}$$

Now, our goal is to find k^* that maximizes (8), where $1 \leq k^* \leq n-2$. Let us define a function $f:[1,n-2]\to\mathbb{R}$, where $f(k)=k(n-k)[(n-1)^2-k^2]$. The function f is a polynomial of degree 4, with four simple real zeros $1-n, 0, n-1$, and n. Its derivative has three simple real zeros, which interlace with those of f. As a result, f has exactly one local maximum strictly between 0 and $n-1$. From Lemma 5, we know that this maximum cannot exceed $\lfloor n/2\rfloor$. Therefore, we seek the largest $k\in[1,\lfloor n/2\rfloor-1]$ for which $f(k)\leq f(k+1)$. The latter inequality is equivalent to

$$k(n-k)[(n-1)^2-k^2]\leq(k+1)(n-k-1)[(n-1)^2-(k+1)^2],$$

which is, after simplification, equivalent to

$$4k^2+(n+2)k-n(n-2)\leq 0. \tag{9}$$

By solving the quadratic inequality (9) on the interval $[1,\lfloor n/2\rfloor-1]$, we obtain

$$1\leq k\leq\frac{1}{8}\left[\sqrt{17n^2-28n+4}-(n+2)\right].$$

If the expression under the square root is not a complete square, then the term in square brackets is not an integer, and hence (8) attains its unique maximum integer value for

$$k^*=\left\lfloor\frac{1}{8}\left[\sqrt{17n^2-28n+4}-(n+2)\right]\right\rfloor+1$$

$$= \left\lfloor \frac{1}{8} \left[\sqrt{17n^2 - 28n + 4} - (n-6) \right] \right\rfloor .$$

If, on the other hand, $17n^2 - 28n + 4 = s^2$ for some nonnegative integer s, then the expression in square brackets becomes an integer. If, in addition, both s and $n-6$ have the same remainder when divided by 8, then the term in the square brackets is divisible by 8, and the result is an integer k^* such that $f(k^*) = f(k^*+1)$. Hence, both k^* and k^*+1 will yield maximizing graphs. Since f is a polynomial of degree 4, it is clear that its restriction on positive integers cannot achieve its local maximum at more than 2 consecutive integer values. Hence, G must be either $CS_{k^*,n-k^*}$ or $CS_{k^*+1,n-k^*-1}$. ■

The problem of characterizing the values of n for which the maximum occurs at two consecutive integer values of k remains unresolved. We will discuss this issue further in the next section.

For large values of n, the ratio k^*/n becomes arbitrarily close to $\frac{\sqrt{17}-1}{8}$ $\approx 0.3903882032n$, confirming thus the approximate linear relation conjectured by the authors of [4].

We observe that the optimal k for $l = 2$ is larger than the one for $l = 1$. It is natural to wonder if this trend continues for $l > 2$. In the general case, for $l > 2$, explicit formulas like the ones derived for $l = 2$ are unlikely to exist. Instead, we can attempt to estimate the position of the optimal k for large values of l and n by considering a continuous relaxation of the problem.

So, let $f(x) = x(n-x)[(n-1)^l - x^l]$ be the continuous relaxation of $f(k) = cM_l(K_k + \overline{K}_{n-k})$. Clearly, f is a polynomial of degree l with a positive leading coefficient. Depending on the parity of l, it has either three (for l odd) or four (for l even) simple real zeros. Its derivative, $f'(x)$, is given by

$$f'(x) = (l+2)x^{l+1} - n(l+1)x^l - 2(n-1)^l x + n(n-1)^l. \qquad (10)$$

At this point, we can no longer rely on interlacing to demonstrate that the derivative has exactly one simple real zero in the interval $(1, n-2)$. In order to establish this fact, we must prove several auxiliary results.

Lemma 6. *Function $f'(x)$ has one simple real zero in $(1, n-2)$.*

Proof. Equation $f'(x) = 0$ is equivalent to

$$(l+2)x^{l+1} + n(n-1)^l = n(l+1)x^l + 2(n-1)^l x.$$

Let us denote

$$g(x) = (l+2)x^{l+1} + n(n-1)^l, \qquad h(x) = n(l+1)x^l + 2(n-1)^l x,$$

and consider the equation $g(x) = h(x)$. It is a matter of somewhat tedious, but otherwise straightforward computation, to verify the following claims:
(i) $g(1) > h(1)$, for all $l \geq 1$ and $n \geq 4$;
(ii) $g(n/2) < h(n/2)$, for all $l \geq 1$ and $n \geq 4$;
(iii) $g'(x) < h'(x)$ for all $x \in (1, n/2)$.
Hence, the curve $y = h(x)$ is below the curve $y = g(x)$ at the left endpoint of the interval $[1, n/2]$, ends above the curve $y = g(x)$ at the right endpoint, and grows faster than $y = g(x)$ throughout the entire interval. From the first two claims it follows that $f'(x)$ has opposite signs at the endpoints of the interval $[1, n/2]$, while the third claim ensures that the derivative does not change sign within the interval. Therefore, it must have exactly one simple zero within the considered interval. ■

Note that for large values of l, the first two terms of the function (10) become negligibly small compared to the remaining two terms. As a result, the entire function f' can be viewed as a small perturbation of the simpler function $f_1'(x) = -2(n-1)^l x + n(n-1)^l$. Now the solution of $f'(x) = 0$ must be close to the only solution of $f_1'(x) = 0$, i.e., to $x = \frac{n}{2}$.

We can summarize our analysis in the following corollary.

Corollary 2. *For large values of n and l, the optimal order of the clique in the complete split graphs that maximize $cM_l(G)$ approaches $n/2$.*

5 Concluding remarks

In this paper, we introduced and analyzed a generalized complementary second Zagreb index, a novel index that encompasses a class of indices suitable for use as irregularity measures. Our generalization was inspired by a recent paper by Furtula and Oz, where they investigated a specific case and put forward an interesting conjecture about the structure of graphs that maximize it. We have confirmed the validity of their conjecture and shown that it also applies to the generalized complementary second Zagreb index.

It would be interesting to explore whether our results hold when the nonnegative integers in the definition of $cM_l(G)$ are replaced by more general exponents. While it would be reasonable to expect the results to extend to positive non-integer values of l, negative values of l or those between 0 and 1 may result in different behavior.

Another intriguing direction would be to examine whether the proposed generalization provides new insights compared to the existing ones, essentially conducting an analysis similar to that in the paper by Furtula and Oz.

Finally, several mathematically interesting questions remain open. For instance, when $l = 2$, we are unsure whether there are finitely or infinitely many values of n for which two consecutive integer values of optimal k exist. This situation can only occur when the expression

$$\frac{1}{8}\left[\sqrt{17n^2 - 28n + 4} - (n - 6)\right]$$

of Theorem 1 is an integer, which requires $\sqrt{17n^2 - 28n + 4} - (n - 6)$ to be divisible by 8. It is a straightforward exercise in Diophantine equations to show that there are infinitely many values of n for which $\sqrt{17n^2 - 28n + 4}$ is a nonnegative integer, but not all of them are congruent to $n - 6$ modulo 8. Such values of n seem to be quite rare; apart from the trivial case of $n = 2$, which gives $k = 0$, there are only 8 such values smaller than 10^8, and only 48 smaller than 10^9. The first few interesting cases are $n = 12$, yielding $k = 4$ and $k = 5$ as optimal clique orders, $n = 117$ with $k = 45$ and

$k = 46$, and $n = 450$, leading to optimal values of $k = 175$ and $k = 176$. We are inclined to believe that there are infinitely many such values, and we leave the claim as an open problem for interested readers.

To conclude this section, we explicitly present several open problems:

Problem 1. Characterize trees having maximum and minimum generalized complementary second Zagreb index. Do the extreme trees differ depending on the parameter l?

Problem 2. Characterize unicyclic graphs having maximum and minimum generalized complementary second Zagreb index.

Problem 3. Derive bounds on the generalized complementary second Zagreb index of a graph as functions of its order and diameter.

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