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Article

Ad-Hoc Lanzhou Index

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Abstract: This paper initiates the study of the mathematical aspects of the ad-hoc Lanzhou index. If G is a graph with the vertex set $\{x_1, \cdots, x_n\}$, then the ad-hoc Lanzhou index of G is defined by $\overline{Lz}(G) = \sum_{i=1}^{n} d_i(n-1-d_i)^2$, where d_i represents the degree of the vertex x_i. Several identities for the ad-hoc Lanzhou index, involving some existing topological indices are established. The problems of finding graphs with the extremum values of the ad-hoc Lanzhou index from the following sets of graphs are also attacked: (i) set of all connected ξ-cyclic graphs of a fixed order, (ii) set of all connected molecular ξ-cyclic graphs of a fixed order, (iii) set of all graphs of a fixed order, (iv) set of all connected molecular graphs of a fixed order.

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MSC: 05C07; 05C09; 05C92

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1. Introduction

Graph invariants are regarded as the properties of a graph that the graph isomorphism preserves [1]. Real-valued graph invariants are often known as topological indices [3]. We mention [2–5] as sources for terminology and notations related to (chemical) graph theory.

One of the most extensively researched topological indices is the first Zagreb index, which originally appeared in [6]. For a graph G, its first Zagreb index is often represented by $M_1(G)$ and is defined (for example see [7]) as

$$M_1(G) = \sum_{t \in V(G)} (d_t)^2 = \sum_{rs \in E(G)} (d_r + d_s),$$

where d_t represent the degree of the vertex t in G and $E(G)$ is the set of edges of G. The forgotten topological index [8] (which is sometimes referred to as the F-index, see also [9]) is another index that first appeared in [6]. The F-index of a graph G is represented by $F(G)$ and is defined [8] as follows.

$$F(G) = \sum_{t \in V(G)} (d_t)^3 = \sum_{rs \in E(G)} \left((d_r)^2 + (d_s)^2 \right).$$

Vukičević et al. [10] studied (chemically as well as mathematically) the following linear combination of the indices $M_1(G)$ and $F(G)$ for a graph of order n and referred it to as the Lanzhou index:

$$Lz(G) = (n-1)M_1(G) - F(G).$$

The Lanzhou index can be rewritten as

$$Lz(G) = \sum_{t \in V(G)} (d_t)^2 \, \overline{d_t},$$

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where $\overline{G}$ is the complement of G and $\overline{d_t}$ represent the degree of t in $\overline{G}$. The Refs. [11–14] provide some recent extremal results regarding the Lanzhou index.

If $TI(G)$ is a topological index of a graph G, then $TI(L(G))$ is known as its reformulated version [15,16]. Here, $L(G)$ means the line graph of G. Motivated by the concept of reformulated topological indices [15,16], we consider ad-hoc topological indices: if $TI(G)$ is a topological index of a graph G, then we call $TI(\overline{G})$ as the ad-hoc version of $TI(G)$, where $\overline{G}$ represents the complement of G. Thus, applying the idea of ad-hoc topological indices on the Lanzhou index gives the ad-hoc Lanzhou index, represented by $\widetilde{Lz}$. The ad-hoc Lanzhou index [10], for a graph G, is defined as

$$\widetilde{Lz}(G) = \sum_{t \in V(G)} d_t \left(\overline{d_t}\right)^2 = Lz(\overline{G}).$$

If $|V(G)| = n$, then $\overline{d_t} = n - d_t - 1$ and thus

$$Lz(G) = \sum_{t \in V(G)} \left(d_t\right)^2 \left(n - d_t - 1\right) \quad \text{and} \quad \widetilde{Lz}(G) = \sum_{t \in V(G)} d_t \left(n - d_t - 1\right)^2.$$

The ad-hoc Lanzhou index was examined in [10] for predicting the octanol-water partition coefficient of nonane isomers and it was found that this index performs better than both the well-known first Zagreb index and the F-index.

A graph with n vertices is called an n-order graph. Molecular graphs are those with the maximum degree at most 4. A connected ξ-cyclic graph of order n is a connected n-order graph with $\xi + n - 1$ edges. For $\xi = 0, 1, 2,$ and 3, a connected ξ-cyclic graph is also known as a tree, connected unicyclic graph, connected bicyclic graph, and connected tricyclic graph, respectively.

In this paper, several identities for the ad-hoc Lanzhou index, involving some existing topological indices are established. The problems of finding graphs with the extremum values of the ad-hoc Lanzhou index from the following sets of graphs are also attacked: (i) set of all n-order connected ξ-cyclic graphs (with a particular emphasis on unicyclic graphs, trees, bicyclic as well as tricyclic graphs), (ii) set of all n-order connected molecular ξ-cyclic graphs, (iii) set of all n-order graphs, (iv) set of all n-order connected molecular graphs.

2. Identities

For a graph G, its forgotten topological coindex (or simply the F-coindex) is represented by $\overline{F}$ and is defined [17,18] by

$$\overline{F}(G) = \sum_{st \notin E(G)} \left(\left(d_s\right)^2 + \left(d_t\right)^2\right).$$

Actually, the F-coindex is equal to the Lanzhou index for every graph, see for example [19]. Generally, if $\sum_{st \in E(G)} f(g(s), g(t))$ is a topological index of a graph G then the corresponding coindex is defined as $\sum_{st \notin E(G)} f(g(s), g(t))$, where g maybe the degree, the eccentricity, or any other (real-valued) parameter defined on the vertices of G and f is a real-valued symmetric function. Note that the Lanzhou index can be rewritten as

$$Lz(G) = \sum_{st \in E(G)} \left(d_s(G) d_s(\overline{G}) + d_t(G) d_t(\overline{G})\right),$$

where $d_s(G)$ and $d_s(\overline{G})$ indicate the degrees of the vertex $s \in V(G)$ in G and $\overline{G}$, respectively. When there is no chance of confusion, we drop "(G)" from the notation $d_s(G)$. Applying the definition of a coindex to the Lanzhou index yields the Lanzhou coindex $\overline{Lz}$:

$$\overline{Lz}(G) = \sum_{st \notin E(G)} \left(d_s(G) d_s(\overline{G}) + d_t(G) d_t(\overline{G})\right).$$

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Consequently, we have

$$\overline{Lz}(G) = \sum_{st\in E(\overline{G})} \left(d_s(\overline{G})d_s(G) + d_t(\overline{G})d_t(G)\right) = Lz(\overline{G}).$$

The following result is immediate from the above.

Observation 1. *For every graph G, its Lanzhou coindex is equal to the Lanzhou index of $\overline{G}$ (which is termed as the ad-hoc Lanzhou index of G), which is equal to the F-coindex of $\overline{G}$; that is,*

$$\overline{Lz}(G) = Lz(\overline{G}) = \widetilde{Lz}(G) = \overline{F}(\overline{G}). \tag{1}$$

Because of (1), the identity given in the following proposition is already known (see Equation (3.6) in [18]); however, here we provide its more simple proof.

Proposition 1. *For any graph G with size m and order n, the following identity holds*

$$\widetilde{Lz}(G) = 2(n-1)^2m + F(G) - 2(n-1)M_1(G).$$

Proof. Note that the formula for $\widetilde{Lz}$ can be rewritten as

$$\widetilde{Lz}(G) = \sum_{rs\in E(G)} \left((n-d_r-1)^2 + (n-d_s-1)^2\right). \tag{2}$$

Expanding the squared terms in (2) and then making use of the definitions of F and M_1, we get the desired identity. □

By Proposition 1, every upper bound on M_1 provides a lower bound on $\widetilde{Lz}$ and every lower bound on M_1 gives an upper bound on $\widetilde{Lz}$; many bounds on M_1 can be found in [7]. Also, from the aforementioned proposition, it is concluded that every lower/upper bound on F provides a(n) lower/upper bound on $\widetilde{Lz}$, respectively; several bounds on F-index can be found in [20].

Proposition 2. *For any graph G with size m and order n, the following identity holds*

$$\widetilde{Lz}(G) = 2(n-1)^2m - Lz(G) - (n-1)M_1(G)$$

Proof. The identity given in Proposition 1 gives the desired result after utilizing the following well-known trivial formula:

$$Lz(G) = (n-1)M_1(G) - F(G).$$

□

By Proposition 2, every upper bound on Lz provides a lower bound on $\widetilde{Lz}$ and every lower bound on Lz gives an upper bound on $\widetilde{Lz}$; considerable number of bounds on Lz can be found in [20].

3. Extremal Results Concerning ξ-Cyclic Graphs

If $st \in E(G)$ and $rt \notin E(G)$ then let $G - st + rt$ denote the graph formed from G by removing the edge st and adding the edge rt. We begin this section by providing the following simple but useful lemma that will be used frequently in the remaining part of this paper:

Lemma 1. *Suppose that G is an n-order graph containing r, s, t, such that $rt \notin E(G)$ and $st \in E(G)$. If $G^* = G - st + rt$, then*

$$\widetilde{Lz}(G) - \widetilde{Lz}(G^*) = \big((n-4) + 3(n-d_r-d_s)\big)(d_r - d_s + 1),$$

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where $d_r = d_r(G)$ *and* $d_s = d_s(G)$.

Proof. Utilizing the definition of $\widetilde{Lz}$, we get

$$\begin{aligned}\widetilde{Lz}(G) - \widetilde{Lz}(G^*) =& d_r(n-d_r-1)^2 + d_s(n-d_s-1)^2 \\ & -(d_r+1)(n-d_r-2)^2 - (d_s-1)(n-d_s)^2 \\ =& \big((n-4)+3(n-d_r-d_s)\big)(d_r-d_s+1).\end{aligned}$$

□

Lemma 2. *Let G be an n-order graph containing a path rst such that* $rt \notin E(G)$ *and the edge rs does not lie on any cycle of length 3, where* $d_r(G) \geq d_s(G)$ *and* $n \geq 5$. *If* $G^* = G - st + rt$, *then*

$$\widetilde{Lz}(G) > \widetilde{Lz}(G^*).$$

Proof. By Lemma 1 we get

$$\widetilde{Lz}(G) - \widetilde{Lz}(G^*) = \big((n-4)+3(n-d_r-d_s)\big)(d_r-d_s+1), \tag{3}$$

where $d_r = d_r(G)$ and $d_s = d_s(G)$. Since the edge rs does not lie on any cycle of length 3, we have $n - d_r - d_s \geq 0$ and thus under the given constraints, Equation (3) gives

$$\widetilde{Lz}(G) - \widetilde{Lz}(G^*) > 0.$$

□

Now, we provide the first extremal result involving the minimum possible value of $\widetilde{Lz}$ for trees.

Theorem 1. *In the set of all n-order trees, with* $n \geq 5$, *only the star graph* S_n *possesses the lowest value of* $\widetilde{Lz}$; *the mentioned lowest value is* $(n-1)(n-2)^2$.

Proof. Let T be a tree possessing the lowest value of $\widetilde{Lz}$ in the set of all n-order trees. Suppose on the contrary that $T \neq S_n$. Then $\Delta(T) \neq n-1$. Consider a path rst of T such that $d_r(T) \geq d_s(T)$. If T^* is the graph deduced from T by dropping st and inserting rt, then by Lemma 2 we have

$$\widetilde{Lz}(T) > \widetilde{Lz}(T^*),$$

a contradiction. Also, by elementary computations, one has

$$\widetilde{Lz}(S_n) = (n-1)(n-2)^2.$$

□

Next, we pay attention to deriving extremal results involving the minimum possible value of $\widetilde{Lz}$ for connected ξ-cyclic graphs. For this, we require the next two results.

Lemma 3. *If G is an n-order connected* ξ*-cyclic graph, rs is an edge of G and* γ *is the number of common neighbors of s and r, then* $d_r + d_s \leq n + \gamma \leq n + \xi$.

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Proof. Let α be the number of those neighbors of r that are neither adjacent to s nor equal to s; see Figure 1. Let β be the number of those neighbors of s that are neither adjacent to r nor equal to r. Then $d_r = \alpha + \gamma + 1$ and $d_s = \beta + \gamma + 1$. Note that $\alpha + \beta + \gamma \leq n - 2$ and $\gamma \leq \xi$. Thus,

$$d_r + d_s = \alpha + \beta + 2\gamma + 2 \leq n + \gamma \leq n + \xi.$$

□

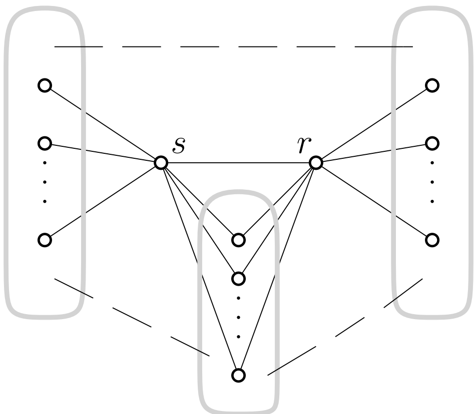

Figure 1. The structure of the graph G used in Lemma 3.

Lemma 4. *Suppose that G is a connected ξ-cyclic graph of order n containing a path rst such that $rt \notin E(G)$, where $d_r(G) \geq d_s(G)$ and $n \geq 3\xi + 5$. If $G^* = G - st + rt$, then*

$$\widetilde{Lz}(G) > \widetilde{Lz}(G^*).$$

Proof. In the following, we take $d_r = d_r(G)$ and $d_s = d_s(G)$. By Lemma 3, the inequality $n - d_r - d_s \geq -\xi$ holds and thus under the given constraints, Lemma 1 yileds

$$\widetilde{Lz}(G) - \widetilde{Lz}(G^*) = \big((n-4) + 3(n - d_r - d_s)\big)(d_r - d_s + 1) > 0.$$

□

Corollary 1. *Let G be a graph possessing the lowest value of $\widetilde{Lz}$ in the set of all n-order connected ξ-cyclic graph, with $n \geq 3\xi + 5$. Then $\Delta(G) = n - 1$.*

Proof. Contrarily, assume that $\Delta(G) \neq n - 1$. Take a vertex $r \in V(G)$ satisfying $d_r(G) = \Delta(G)$. Then G has a path rst such that $rt \notin E(G)$. Take $G^* = G - st + rt$. By Lemma 4, it holds that $\widetilde{Lz}(G) > \widetilde{Lz}(G^*)$, which is not possible because of the definition of G. Thus, $\Delta(G) = n - 1$. □

Next, we provide extremal results involving the minimum possible values of $\widetilde{Lz}$ for connected ξ-cyclic graphs when $1 \leq \xi \leq 5$. For $\xi = 1, 2, \ldots, 5$, connected ξ-cyclic graphs are also known as unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic.

Note that there are only two (non-isomorphic) 4-order connected unicyclic graphs and both of them have the same value of $\widetilde{Lz}$. Thus, in the next theorem, we find the extremal graphs of order at least 5.

Theorem 2. *The graph generated from the n-order start graph S_n by inserting an edge, solely possesses the lowest value of $\widetilde{Lz}$ in the set of all n-order connected unicyclic graphs, for every $n \geq 8$. For $n = 7, 6, 5$, the extremal graphs are depicted in the first row, second row, third row of Figure 2, respectively.*

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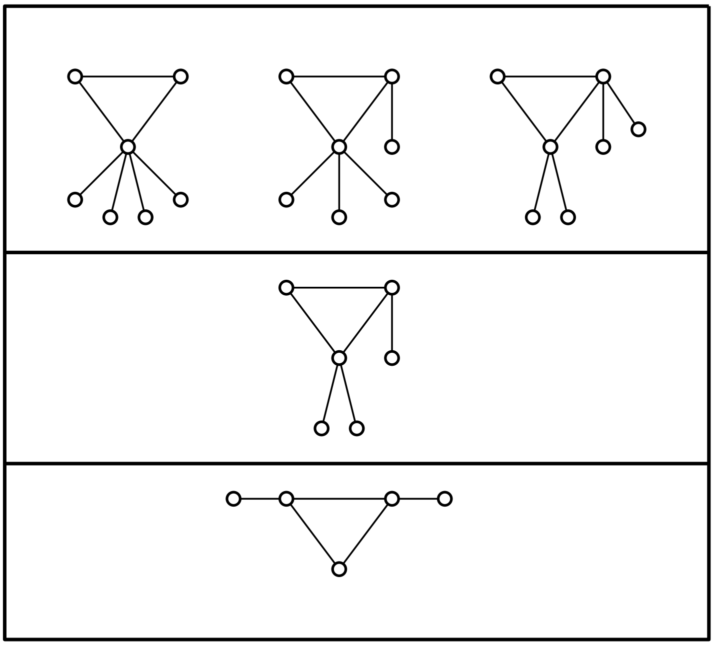

Figure 2. The graphs possessing the lowest value of $\widetilde{Lz}$ in the set of all n-order connected unicyclic graphs, for $n = 5, 6, 7$.

Proof. Since there is only one n-order unicyclic graph of maximum degree $n-1$ for every $n \geq 8$, the desired conclusion follows from Corollary 1 for $n \geq 8$. Lemma 2 implies that if G is a graph possessing the least value of $\widetilde{Lz}$ in the set of all n-order connected unicyclic graphs, with $n \geq 5$, then the number of pendent vertices in G becomes $n-3$. Simple calculations yield the desired conclusion for $n = 5, 6, 7$. □

For $n \geq 5$, denote by $B_n^{(1)}(\eta_1, \eta_2, \eta_3, \eta_4)$ the n-order bicyclic graph shown in Figure 3, where $\eta_1 + \eta_2 + \eta_3 + \eta_4 = n - 4$ with $\eta_1 \geq \eta_4 \geq 0$ and $\eta_2 \geq \eta_3 \geq 0$. Also, for $n \geq 5$, denote by $B_n^{(2)}(\eta_1, \eta_2, \eta_3, \eta_4, \eta_5)$ the n-order bicyclic graph shown in Figure 4, where $\eta_1 + \eta_2 + \eta_3 + \eta_4 + \eta_5 = n - 5$ with $\eta_1 \geq \max\{\eta_2, \eta_3, \eta_4\}$ and $\eta_i \geq 0$ for every $i \in \{1, 2, \ldots, 5\}$.

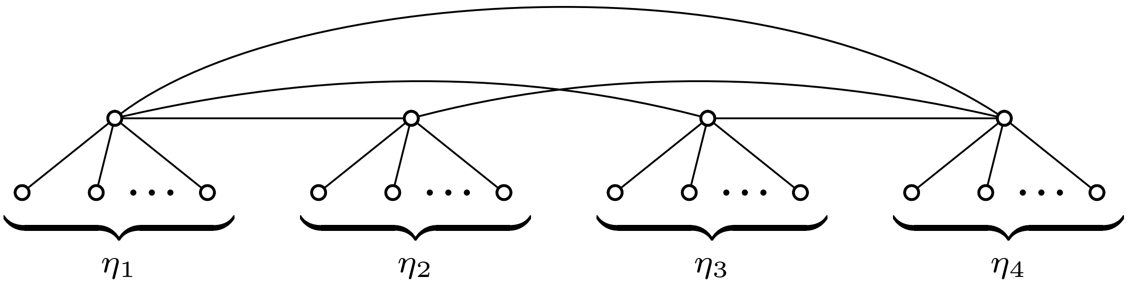

Figure 3. The n-order bicyclic graph $B_n^{(1)}(\eta_1, \eta_2, \eta_3, \eta_4)$, where $\eta_1 + \eta_2 + \eta_3 + \eta_4 = n - 4 \geq 1$ with $\eta_1 \geq \eta_4 \geq 0$ and $\eta_2 \geq \eta_3 \geq 0$.

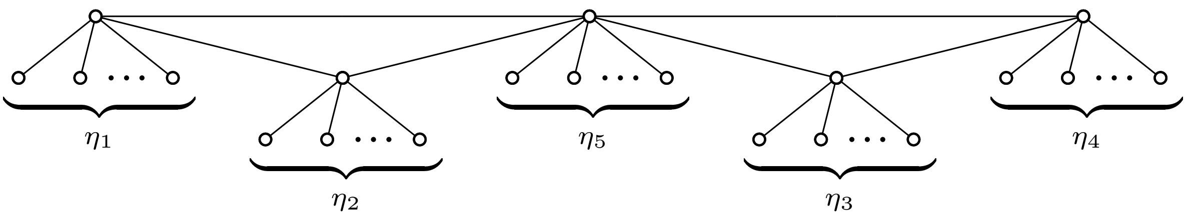

Figure 4. The n-order bicyclic graph $B_n^{(2)}(\eta_1, \eta_2, \eta_3, \eta_4, \eta_5)$, where $\eta_1 + \eta_2 + \eta_3 + \eta_4 + \eta_5 = n - 5 \geq 0$ with $\eta_1 \geq \max\{\eta_2, \eta_3, \eta_4\}$ and $\eta_i \geq 0$ for every $i \in \{1, 2, \ldots, 5\}$.

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Theorem 3. *Considering the family of all n-order bicyclic connected graphs having $n \geq 11$, only the graph $B_n^{(1)}(n-4,0,0,0)$ possesses the lowest value of $\widetilde{Lz}$.*

Proof. Let B_n be an n-order connected bicyclic graph, with $n \geq 11$. If $\Delta(B_n) \neq n-1$ then Corollary 1 implies that B_n cannot possess the lowest value of $\widetilde{Lz}$ in the set of all n-order connected bicyclic graph. If $\Delta(B_n) = n-1$ then $B_n \in \{B_n^{(1)}(n-4,0,0,0), B_n^{(2)}(0,0,0,0,n-5)\}$. By elementary calculations, we verify that the inequality

$$\widetilde{Lz}\left(B_n^{(1)}(n-4,0,0,0)\right) < \widetilde{Lz}\left(B_n^{(2)}(0,0,0,0,n-5)\right)$$

holds for $n \geq 11$. Hence, for every $n \geq 11$, it holds that

$$\widetilde{Lz}(B_n) > \widetilde{Lz}(B_n^{(1)}(n-4,0,0,0)) \quad \text{whenever } B_n \neq B_n^{(1)}(n-4,0,0,0).$$

□

Next, we characterize the graphs possessing the lowest value of $\widetilde{Lz}$ from the set of graphs mentioned in Theorem 3 for $5 \leq n \leq 10$.

Theorem 4. *Let B_n be an n-order connected bicyclic graph with $n \geq 8$ such that the cycles of B_n do not share any edge and $\Delta(B_n) \neq n-1$. Then, B_n does not possess the lowest value of $\widetilde{Lz}$ in the set of all n-order connected bicyclic graphs for every $n \geq 8$.*

Proof. Take a vertex $r \in V(B_n)$ satisfying $d_r(B_n) = \Delta(B_n)$. Since $\Delta(B_n) \neq n-1$, the graph B_n has a path rst such that $rt \notin E(B_n)$. Form a new graph B_n^* from B_n by dropping st and inserting rt. By Lemma 3, the inequality $n - d_r(B_n) - d_s(B_n) \geq -1$ holds and thus by bearing in mind the given assumptions and Lemma 1, we get

$$\begin{aligned}&\widetilde{Lz}(B_n) - \widetilde{Lz}(B_n^*)\\ =&\Big((n-4) + 3\big(n - d_r(B_n) - d_s(B_n)\big)\Big)\Big(d_r(B_n) - d_s(B_n) + 1\Big) > 0,\end{aligned}$$

which implies that B_n cannot possess the lowest value of $\widetilde{Lz}$ in the set of all n-order connected bicyclic graphs for every $n \geq 8$. □

Lemma 2 implies the next corollary.

Corollary 2. *If G is a graph possessing the least value of $\widetilde{Lz}$ in the set of all n-order connected bicyclic graphs, with $n \geq 5$, then G is isomorphic to either $B_n^{(1)}(\eta_1,\eta_2,\eta_3,\eta_4)$ or $B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)$ (see Figures 3 and 4).*

Lemma 5. *For the n-order bicyclic graph $B_n^{(1)}(\eta_1,\eta_2,\eta_3,\eta_4)$ (depicted in Figure 3) with $\eta_2 \geq \eta_3 \geq 1$ and $n \geq 6$, the following inequality holds:*

$$\widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2+1,\eta_3-1,\eta_4)) < \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,\eta_3,\eta_4)).$$

Proof. Since $\eta_1+\eta_2+\eta_3+\eta_4 = n-4$ with $\eta_1 \geq \eta_4 \geq 0$, it holds that $\eta_2+\eta_3 \leq n-4$. Therefore, by bearing in mind the given assumptions and Lemma 1, we get

$$\begin{aligned}&\widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,\eta_3,\eta_4)) - \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2+1,\eta_3-1,\eta_4))\\ =&\big((n-4)+3(n-\eta_2-\eta_3-4)\big)(\eta_2-\eta_3+1) > 0.\end{aligned}$$

□

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Lemma 6. *For the n-order bicyclic graph $B_n^{(1)}(\eta_1,\eta_2,0,\eta_4)$ (depicted in Figure 3) with $\eta_1 \geq \eta_4 \geq 1$ and $6 \leq n \leq 10$, it holds that*

$$\widetilde{Lz}(B_n^{(1)}(\eta_1+1,\eta_2,0,\eta_4-1)) \begin{cases} = \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,\eta_4)) & \text{if either } \eta_2 = 1 \text{ and } n = 7, \\ & \text{or } \eta_2 = 0 \text{ and } n = 10, \\ < \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,\eta_4)) & \text{if } \eta_2 \geq 1 \text{ and } 8 \leq n \leq 10, \\ > \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,\eta_4)) & \text{if } \eta_2 = 0 \text{ and } 6 \leq n \leq 9. \end{cases}$$

Proof. By Lemma 1, we get

$$\begin{aligned} &\widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,\eta_4)) - \widetilde{Lz}(B_n^{(1)}(\eta_1+1,\eta_2,0,\eta_4-1)) \\ =&\big((n-4)+3(n-\eta_1-\eta_4-6)\big)(\eta_1-\eta_4+1). \end{aligned} \quad (4)$$

If $\eta_2 \geq 1$ then the equation $\eta_1+\eta_2+\eta_4 = n-4$ gives $\eta_1+\eta_4 \leq n-5$ (and hence $n \geq 7$; if $n = 7$ then $\eta_1 = \eta_2 = \eta_4 = 1$) and thus under the given constraints Equation (4) yields

$$\widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,\eta_4)) - \widetilde{Lz}(B_n^{(1)}(\eta_1+1,\eta_2,0,\eta_4-1)) \begin{cases} = 0 & \text{if } n = 7, \\ > 0 & \text{if } 8 \leq n \leq 10. \end{cases}$$

If $\eta_2 = 0$ then $\eta_1+\eta_4 = n-4$ and thus Equation (4) yields the desired conclusion. □

Lemma 7. *For the n-order bicyclic graph $B_n^{(1)}(\eta_1,\eta_2,0,0)$ with $n \geq 6$, the following relations hold:*

$$\widetilde{Lz}(B_n^{(1)}(\eta_1+1,\eta_2-1,0,0)) \begin{cases} < \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) & \text{if } \eta_1 \geq \eta_2-1 \geq 0 \text{ and } n \geq 8, \\ = \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) & \text{if either } n = 7 \text{ and } \eta_2 \geq 1, \\ & \text{or } \eta_1 = \eta_2-2 \text{ and } \eta_2 \geq 1, \\ > \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) & \text{if either } \eta_2 = \eta_1 = 1 \text{ and } n = 6, \\ & \text{or } \eta_1 < \eta_2-2 \text{ and } n \geq 8. \end{cases}$$

and

$$\widetilde{Lz}(B_n^{(1)}(\eta_1-1,\eta_2+1,0,0)) \begin{cases} < \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) & \text{if either } \eta_2-1 \geq \eta_1 \geq 1 \text{ and } n \geq 8, \\ & \text{or } \eta_2 = 0,\ \eta_1 = 2 \text{ and } n = 6, \\ = \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) & \text{if either } n = 7 \text{ and } \eta_1 \geq 1, \\ & \text{or } \eta_2 = \eta_1 \geq 1, \\ > \widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) & \text{or } \eta_2 < \eta_1 \text{ and } n \geq 8. \end{cases}$$

Proof. Since $\eta_1+\eta_2 = n-4$, we have

$$\widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) - \widetilde{Lz}(B_n^{(1)}(\eta_1+1,\eta_2-1,0,0)) = \qquad (n-7)(\eta_1-\eta_2+2)$$

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and

$$\widetilde{Lz}(B_n^{(1)}(\eta_1,\eta_2,0,0)) - \widetilde{Lz}(B_n^{(1)}(\eta_1-1,\eta_2+1,0,0)) = (n-7)(\eta_2-\eta_1),$$

which yield the desired relations. □

Lemma 8. *For the n-order bicyclic graph $B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)$ (depicted in Figure 4) with $n \geq 7$, the following inequalities hold:*

$$\widetilde{Lz}(B_n^{(2)}(\eta_1+1,\eta_2,\eta_3,\eta_4-1,\eta_5)) < \widetilde{Lz}(B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)) \text{ when } \eta_4 \geq 1,$$

$$\widetilde{Lz}(B_n^{(2)}(\eta_1+1,\eta_2,\eta_3-1,\eta_4,\eta_5)) < \widetilde{Lz}(B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)) \text{ when } \eta_3 \geq 1,$$

$$\widetilde{Lz}(B_n^{(2)}(\eta_1+1,\eta_2-1,\eta_3,\eta_4,\eta_5)) < \widetilde{Lz}(B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)) \text{ when } \eta_2 \geq 1,$$

Proof. Since $\eta_1+\eta_2+\eta_3+\eta_4+\eta_5 = n-5$ with $\eta_i \geq 0$ for $i \in \{1,2,\ldots,5\}$, it holds that $\eta_1+\eta_j \leq n-5$ for every $j \in \{2,\ldots,5\}$. Also, we recall that $\eta_1 \geq \max\{\eta_2,\eta_3,\eta_4\}$. Therefore, by using the given constraints, we have

$$\begin{aligned}&\widetilde{Lz}(B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)) - \widetilde{Lz}(B_n^{(2)}(\eta_1+1,\eta_2-1,\eta_3,\eta_4,\eta_5))\\ =&((n-4)+3(n-\eta_1-\eta_2-4))(\eta_1-\eta_2+1) > 0,\end{aligned}$$

$$\begin{aligned}&\widetilde{Lz}(B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)) - \widetilde{Lz}(B_n^{(2)}(\eta_1+1,\eta_2,\eta_3-1,\eta_4,\eta_5))\\ =&((n-4)+3(n-\eta_1-\eta_3-4))(\eta_1-\eta_3+1) > 0,\end{aligned}$$

$$\begin{aligned}&\widetilde{Lz}(B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5)) - \widetilde{Lz}(B_n^{(2)}(\eta_1+1,\eta_2,\eta_3,\eta_4-1,\eta_5))\\ =&((n-4)+3(n-\eta_1-\eta_4-4))(\eta_1-\eta_4+1) > 0.\end{aligned}$$

□

Lemma 9. *For the n-order bicyclic graph $B_n^{(2)}(\eta_1,0,0,0,\eta_5)$, the following relations hold:*

$$\widetilde{Lz}(B_n^{(2)}(\eta_1-1,0,0,0,\eta_5+1)) \begin{cases} < \widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) & \text{if } 1 \leq \eta_1 \leq \eta_5+2 \text{ and } n \geq 8, \\ = \widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) & \text{if either } n = 7 \text{ and } \eta_1 \geq 1, \\ & \text{or } \eta_5+3 = \eta_1 \geq 1, \\ > \widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) & \text{if } \eta_1 = 1, \eta_5 = 0 \text{ and } n = 6, \\ & \text{or } \eta_5+3 < \eta_1 \text{ and } n \geq 8. \end{cases}$$

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and

$$\widetilde{Lz}(B_n^{(2)}(\eta_1+1,0,0,0,\eta_5-1)) \begin{cases} < \widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) & \text{if } \eta_1-2 \geq \eta_5 \geq 1 \text{ and } n \geq 8, \\ & \text{or } \eta_1=0,\ \eta_5=1 \text{ and } n=6, \\ = \widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) & \text{if either } n=7 \text{ and } \eta_5 \geq 1, \\ & \text{or } \eta_1-1=\eta_5 \geq 1, \\ > \widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) & \text{if } \eta_5 \geq 1,\ \eta_1-1<\eta_5 \text{ and } n \geq 8. \end{cases}$$

Proof. Since $\eta_1+\eta_5=n-5$, we have

$$\widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) - \widetilde{Lz}(B_n^{(2)}(\eta_1-1,0,0,0,\eta_5+1)) = (n-7)(\eta_5-\eta_1+3)$$

and

$$\widetilde{Lz}(B_n^{(2)}(\eta_1,0,0,0,\eta_5)) - \widetilde{Lz}(B_n^{(2)}(\eta_1+1,0,0,0,\eta_5-1)) = (n-7)(\eta_1-\eta_5-1),$$

from which the required relations follow. □

Denote by K_4-e the graph deduced from the 4-order complete graph K_4 by dropping an edge. Let $B_{n;\alpha}$ be the graph formed from K_4-e by connecting α pendent vertices with one vertex having degree 3 and the rest $n-4-\alpha$ pendent vertices with the other vertex having degree 3 (see the graph placed on the left-hand side in Figure 5), where $0 \leq \alpha \leq \lfloor (n-4)/2 \rfloor$. Let B_n^* denote the graph generated from K_4-e by attaching $n-4$ pendent vertices to a vertex of degree 2 (see the graph placed on the right-hand side in Figure 5). Certainly, $B_{n;0}=B_n^{(1)}(n-4,0,0,0)$.

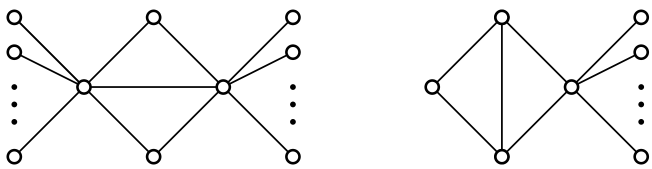

Figure 5. The n-order bicyclic graphs $B_{n;\alpha}$ (on the left side) and B_n^* (on the right side), where $0 \leq \alpha \leq \lfloor (n-4)/2 \rfloor$.

Now, we are in the position to characterize the graphs possessing the lowest value of $\widetilde{Lz}$ from the set of graphs mentioned in Theorem 3 for $5 \leq n \leq 10$.

Theorem 5. *Among all n-order connected bicyclic graphs,*

(i) *only the graph* $B_n^{(1)}(0,n-4,0,0)$ *has the minimum value of* $\widetilde{Lz}$ *for* $n=5$,
(ii) *only the graph* $B_{n;1}$ *has the minimum value of* $\widetilde{Lz}$ *for each* $n \in \{6,7\}$,
(iii) *only the graph* $B_{n;2}$ *has the minimum value of* $\widetilde{Lz}$ *for each* $n \in \{8,9\}$,
(iv) *only the graphs* $B_{n;0}, B_{n;1}, B_{n;2}, B_{n;3}$ *have the minimum value of* $\widetilde{Lz}$ *for* $n=10$.

Proof. By Corollary 2, it is enough to investigate the values of $\widetilde{Lz}$ for the graphs:

$$B_n^{(1)}(\eta_1,\eta_2,\eta_3,\eta_4) \quad \text{and} \quad B_n^{(2)}(\eta_1,\eta_2,\eta_3,\eta_4,\eta_5).$$

For $n = 5$, there are only three such graphs; namely, $B_n^{(1)}(n-4,0,0,0)$, $B_n^{(1)}(0,n-4,0,0)$ and $B_n^{(2)}(0,0,0,0,n-5)$. Certainly, for $n=5$, it holds that

$$\widetilde{Lz}(B_n^{(1)}(0,n-4,0,0)) < \widetilde{Lz}(B_n^{(1)}(n-4,0,0,0)) < \widetilde{Lz}(B_n^{(2)}(0,0,0,0,n-5)),$$

which confirms Part (i) of the theorem.

If G is a graph possessing the least value of $\widetilde{Lz}$ in the set of all 6-order connected bicyclic graphs, then from Lemmas 6, 7, 8 and 9, it follows that $G \in \{G_1, G_2, G_3, G_4\}$ where the graphs G_1, G_2, G_3, G_4, are depicted in Figure 6. It holds that

$$\widetilde{Lz}(G_1) < \widetilde{Lz}(G_2) = \widetilde{Lz}(G_3) \quad \text{and} \quad \widetilde{Lz}(G_1) < \widetilde{Lz}(G_4).$$

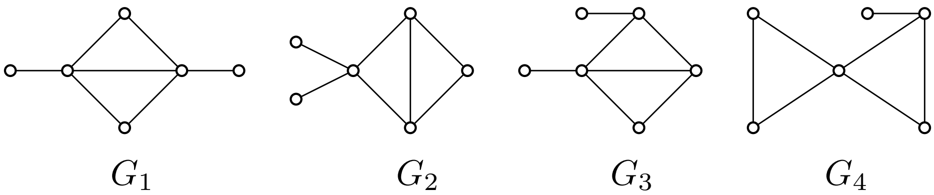

Figure 6. The 6-order connected bicyclic graphs G_1, G_2, G_3 and G_4.

If G is a graph possessing the least value of $\widetilde{Lz}$ in the set of all 7-order connected bicyclic graphs, then from Lemmas 6, 7, 8 and 9, it follows that $G \in \{H_1, H_2, \dots, H_8\}$ where the graphs $H_1, H_2, \dots, H_8$, are depicted in Figure 7. It holds that

$$\widetilde{Lz}(H_1) < \widetilde{Lz}(H_2) = \widetilde{Lz}(H_3) = \widetilde{Lz}(H_5) = \widetilde{Lz}(H_6)$$

and

$$\widetilde{Lz}(H_1) < \widetilde{Lz}(H_4) = \widetilde{Lz}(H_7) = \widetilde{Lz}(H_8).$$

Since $G_1 = B_{6;1}$ and $H_1 = B_{7;1}$, the proof of Part (ii) is completed.

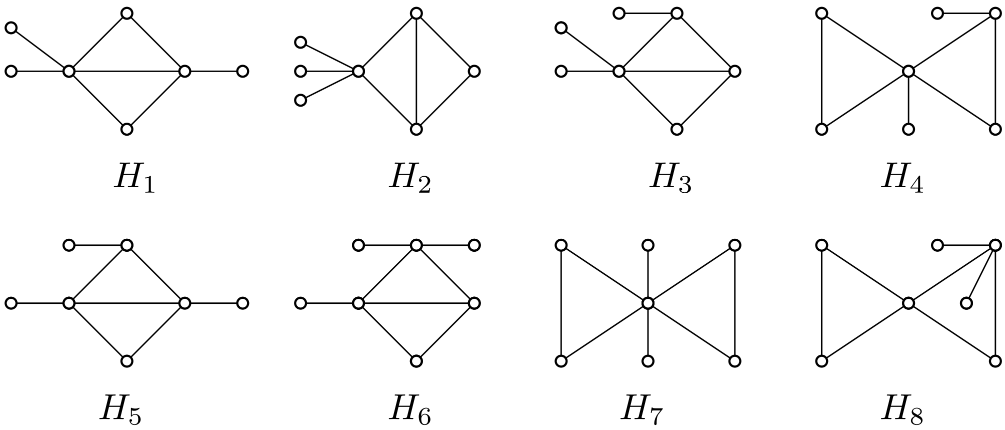

Figure 7. The 7-order connected bicyclic graphs $H_1, H_2, \dots, H_8$.

Theorem 4 states that if B_n is an n-order connected bicyclic graph with $n \geq 8$ such that the cycles of B_n do not share any edge and $\Delta(B_n) \neq n-1$, then B_n does not possess the lowest value of $\widetilde{Lz}$ in the family of all n-order bicyclic connected graphs having $n \geq 8$. Thus, if G is a graph possessing the least

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value of $\widetilde{Lz}$ in the set of all n-order connected bicyclic graphs for $n \in \{8, 9, 10\}$, then from Lemmas 6 and 7 it follows that

$$\begin{cases} G \in \{B_{n;0}, B_{n;2}, B^*_n, B^\dagger_n\} & \text{when } n \in \{8, 9\}, \\ G \in \{B_{n;\alpha}, B^*_n, B^\dagger_n\} & \text{when } n = 10. \end{cases}$$

where $B^\dagger_n = B^{(2)}_n(0, 0, 0, 0, n-5)$. For $n \in \{8, 9, 10\}$ the following relations hold:

$$\begin{aligned} \widetilde{Lz}(B_{n;0}) &= n^3 - n^2 - 28n + 68 \\ &< \widetilde{Lz}(B^*_n) = n^3 - 39n + 96 \\ &< \widetilde{Lz}(B^\dagger_n) = n^3 - n^2 - 24n + 52. \end{aligned}$$

Also, the inequality $\widetilde{Lz}(B_{n;2}) < \widetilde{Lz}(B_{n;0})$ holds for each $n \in \{8, 9\}$. Moreover, the equation $\widetilde{Lz}(B_{10;\alpha}) = 688$ holds for every $\alpha \in \{0, 1, 2, 3\}$. Thus, Parts (iii) and (iv) also hold.
□

Theorem 6. *Considering the family of all n-order tricyclic connected graphs having with $n \geq 14$, only the right-most graph in Figure 8 possesses the lowest value of $\widetilde{Lz}$.*

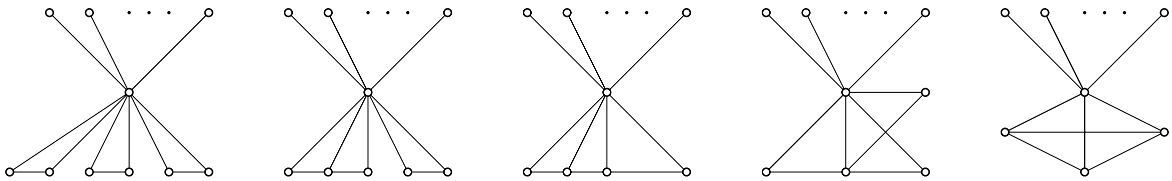

Figure 8. The graphs $J_1, J_2, \ldots, J_5$, (from left to right, respectively) used in Theorem 6.

Proof. Let G be an n-order connected tricyclic graph, with $n \geq 14$. If $\Delta(G) \neq n-1$ then Corollary 1 implies that G cannot possess the lowest value of $\widetilde{Lz}$ in the set of all n-order connected tricyclic graph. If $\Delta(G) = n-1$ then G is one of the graphs $J_1, J_2, \ldots, J_5$ (from left to right, respectively) shown in Figure 8. We have

$$\widetilde{Lz}(J_1) = (n-7)(n-2)^2 + 12(n-3)^2,$$

$$\widetilde{Lz}(J_2) = (n-6)(n-2)^2 + 8(n-3)^2 + 3(n-4)^2,$$

$$\widetilde{Lz}(J_3) = (n-5)(n-2)^2 + 4(n-3)^2 + 6(n-4)^2,$$

$$\widetilde{Lz}(J_4) = (n-5)(n-2)^2 + 6(n-3)^2 + 4(n-5)^2,$$

$$\widetilde{Lz}(J_5) = (n-4)(n-2)^2 + 9(n-4)^2.$$

But, $\widetilde{Lz}(J_i) > \widetilde{Lz}(J_5)$ for every $i \in \{1, 2, 3, 4\}$. Hence, $\widetilde{Lz}(G) \geq \widetilde{Lz}(J_5)$ with equality if and only if $G = J_5$. □

A non-trivial path $P : r_1 \ldots r_p$ of a graph G is said to be a pendent path if

$$\max\{d_{r_1}(G), d_{r_p}(G)\} \geq 3 \quad \text{and} \quad \min\{d_{r_1}(G), d_{r_p}(G)\} = 1,$$

provided that $d_{r_i}(G) = 2$ when $2 \leq i \leq p-1$. By adjacent pendent paths in a graph G, we mean the pendent paths of G having a common vertex.

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Lemma 10. *For $n \geq 5$, if G is a connected n-order graph possessing adjacent pendent paths, then there exists a connected n-order graph G^* which has no adjacent pendent paths satisfying $|E(G)| = |E(G^*)|$ and*

$$\widetilde{Lz}(G) < \widetilde{Lz}(G^*).$$

Proof. Let s be the common vertex of two adjacent pendent paths P_1 and P_2 in G. Assume that the edge st belongs to the path P_1. Let $r \in V(G)$ be the vertex of P_2 satisfying $d_r(G) = 1$. Take $G' = G - st + rt$. Evidently, $|E(G)| = |E(G')|$. Since $n - 4 > 0$ and $n - 1 \geq d_s(G) \geq 3$, by Lemma 1 we get

$$\widetilde{Lz}(G) - \widetilde{Lz}(G') = -\left[n - 4 + 3(n - 1 - d_s(G))\right](d_s(G) - 2) < 0.$$

If G' contains no adjacent pendent paths, the lemma holds true. If G' does contain such paths, we can perform again the above-mentioned transformation successively until we obtain the desired graph G^* satisfying $\widetilde{Lz}(G) < \widetilde{Lz}(G') < \cdots < \widetilde{Lz}(G^*)$. □

The next result is one of the direct outcomes of Lemma 10.

Theorem 7. *In the set of all n-order trees, with $n \geq 5$, only the path graph P_n possesses the highest value of $\widetilde{Lz}$; the mentioned highest value is*

$$2(n - 2)(n^2 - 5n + 7).$$

Lemma 11. *If G is a graph possessing the highest value of $\widetilde{Lz}$ among the family of all n-order connected ξ-cyclic graphs admitting $n \geq 5$ and $\xi \geq 1$, then $\delta(G) > 1$.*

Proof. Contrary, let $\delta(G) = 1$. Because of the constraint $\xi \geq 1$, the graph G must contain at least one pendent path, say P. Let r and s be the terminal end vertices of the path P; particularly, assume that $d_s(G) \geq 3$ and $d_r(G) = 1$. Let $tr \in E(G)$ where t does not belong to the path P. Take $G^* = G - st + rt$. After the same calculations as made in the proof of Lemma 10, we arrive at $\widetilde{Lz}(G) < \widetilde{Lz}(G^*)$; this contradicts the definition of G. Thereby, $\delta(G) > 1$.
□

The next result is one of the direct outcomes of Lemma 11.

Theorem 8. *Considering the family of all n-order unicyclic connected graphs having $n \geq 5$, only the cycle graph C_n possesses the highest value of $\widetilde{Lz}$; the mentioned highest value is $2n(n - 3)^2$.*

Lemma 12. *If G is a graph possessing the highest value of $\widetilde{Lz}$ in the family of all n-order connected ξ-cyclic graphs admitting $n \geq 2(\xi - 1) \geq 2$ and $n \geq 8$, then $\Delta(G) = 3$.*

Proof. The connectedness of G and the constraint $\xi \geq 2$ guaranty that $\Delta(G) \geq 3$. Contrarily, let $\Delta(G) \geq 4$. By Lemma 11, the inequality $\delta(G) \geq 2$ holds.

Suppose that G has m edges. Represent by N_i the number of members of $\{r \in V(G) : d_r(G) = i\}$. Since $\xi = m - n + 1$, the inequality $n \geq 2(\xi - 1)$ yields $n \geq 2(m - n)$, which further implies that

$$\sum_{i=2}^{\Delta(G)} N_i \geq 2\left(\sum_{i=2}^{\Delta(G)} \frac{i\,N_i}{2} - \sum_{i=2}^{\Delta(G)} N_i\right) = 2\left(\sum_{i=3}^{\Delta(G)} \frac{i\,N_i}{2} - \sum_{i=3}^{\Delta(G)} N_i\right),$$

which guaranties that

$$N_2 \geq \sum_{i=4}^{\Delta(G)} (i - 3)N_i;$$

that is, G possess at least one vertex with degree 2.

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Consider a vertex $s \in V(G)$ such that $d_s(G) = \Delta(G)$ (then certainly we have $4 \leq d_s(G) \leq n-1$). Consider also a vertex $r \in V(G)$ having degree 2. The inequality $d_s(G) \geq 4$ confirms the existence of no less than two neighbors of s that are not adjacent to r. We pick from these neighbors of s a vertex t such that the graph $G^* = G - st + rt$ is connected. First, by using Lemma 1 and then by using the inequalities $4 \leq d_s(G) \leq n-1$ and $n \geq 8$, we get

$$\widetilde{Lz}(G) - \widetilde{Lz}(G^*) = -\left[n - 7 + 3(n - 1 - d_s(G))\right](d_s(G) - 3) < 0,$$

which is at odds with the definition of G. Therefore we derive that $\Delta(G) = 3$, as desired. □

Theorem 9. *Consider the set $\mathbb{G}_{n,\xi}$ of all n-order connected ξ-cyclic graphs with $n \geq 2(\xi - 1) \geq 2$ and $n \geq 8$.*

(i). *If $n = 2(\xi - 1)$ then only (the) 3-regular graph(s) possess(es) the highest value of $\widetilde{Lz}$ in $\mathbb{G}_{n,\xi}$.*
(ii). *If $n > 2(\xi - 1)$ then only the graphs with $(\Delta, \delta) = (3, 2)$ possess the highest value of $\widetilde{Lz}$ in $\mathbb{G}_{n,\xi}$.*

Proof. Assume G is a graph possessing the highest value of $\widetilde{Lz}$ in $\mathbb{G}_{n,\xi}$. Then, by Lemmas 11 and 12, it holds that $\delta(G) \geq 2$ and $\Delta(G) = 3$. Thus, we have

$$N_2 + N_3 = n \tag{5}$$

and

$$2N_2 + 3N_3 = 2(n + \xi - 1). \tag{6}$$

where N_i is defined in the proof of Lemma 12.

(i). If $n = 2(\xi - 1)$ then Equations (5) and (6) yield $N_2 = 0$ and thus G is 3-regular.

(ii). If $n > 2(\xi - 1)$ then Equations (5) and (6) imply that $N_2 > 0$ and $N_3 > 0$, as desired. □

One of the implications of Theorem 9 is the following result.

Theorem 10. *Only the graphs with $(\Delta, \delta) = (3, 2)$ possess the highest value of $\widetilde{Lz}$ in the family of all n-order bicyclic connected graphs admitting $n \geq 6$. For $n = 5$, such an extremal graph can be constructed from the star graph through inserting two non-adjacent edges.*

Proof. If $n \geq 8$ then the desired conclusion follows from Theorem 9. If $n \geq 5$ then by Lemma 11, the minimum degree of a graph possessing the highest value of $\widetilde{Lz}$ in the set of all n-order connected bicyclic graphs must be at least 2. If $n = 5$ then there are only three n-order connected bicyclic graphs with minimum degree at least 2; Figure 9 shows all these three graphs together with the values of $\widetilde{Lz}$. Now, in the following, assume that $n \in \{6, 7\}$.

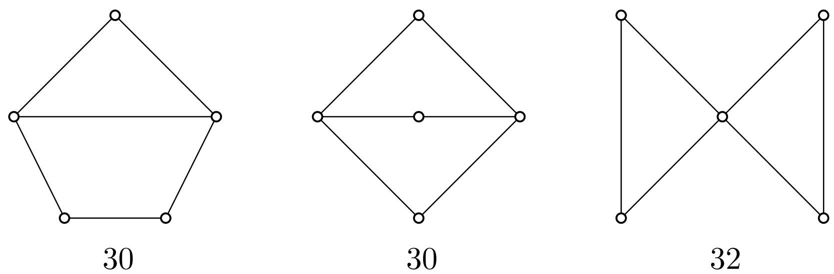

Figure 9. All connected bicyclic graphs of order 5 and minimum degree at least 2, together with the values of $\widetilde{Lz}$.

Assume that G is a graph possessing the highest value of $\widetilde{Lz}$ in the family of all n-order connected bicyclic graphs. Then, by Lemma 11, it holds that $\delta(G) \geq 2$. We claim that $\Delta(G) = 3$. We note that there is no bicyclic graph with $\Delta = n - 1$ and $\delta \geq 2$ (because $n \geq 6$). Thus, from the proof of Lemma

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12 it follows that $\Delta(G) = 3$. Since $n > 2(\xi - 1) = 2$, from the proof of Theorem 9(ii) it follows that $\delta(G) = 2$.
□

Another implication of Theorem 9 is the following theorem.

Theorem 11. *Only the graphs with $(\Delta, \delta) = (3, 2)$ possess the highest value of $\widetilde{Lz}$ in the family of all n-order tricyclic connected graphs admitting $n \geq 8$. For $n = 5$, such an extremal graph can be constructed from the star graph through inserting three edges between one fixed pendent vertex and three other pendent vertices (see the right-most graph in Figure 10). For $n \in \{6, 7\}$, such an extremal graph is the one with minimum degree 2 and maximum degree $n - 1$.*

Proof. If $n \geq 8$ then the desired conclusion follows from Theorem 9. If $n \geq 5$ then by Lemma 11, the minimum degree of a graph possessing the highest value of $\widetilde{Lz}$ in the set of all n-order connected tricyclic graphs must be at least 2. If $n = 5$ then there are only three n-order connected tricyclic graphs with minimum degree at least 2; Figure 10 shows all these three graphs and its caption gives the values of $\widetilde{Lz}$ for the mentioned three graphs. Now, in the following, assume that $n \in \{6, 7\}$.

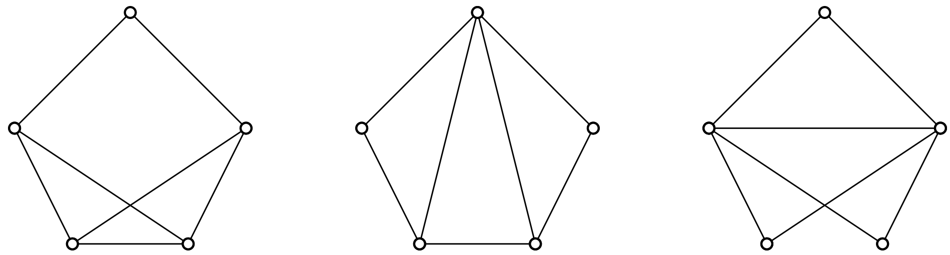

Figure 10. All connected tricyclic graphs of order 5 and minimum degree at least 2. The first, second, and third graphs (from left to right) have the following values of $\widetilde{Lz}$, respectively: 20, 22, and 24.

Assume that G is a graph possessing the highest value of $\widetilde{Lz}$ in the family of all n-order tricyclic connected graphs. Then, by Lemma 11, it holds that $\delta(G) \geq 2$. We claim that $\Delta(G) = n - 1$. Contrarily, let $\Delta(G) < n - 1$. Then from the proof of Lemma 12, it follows that $\Delta(G) = 3$. Since $n > 2(\xi - 1) = 4$, from the proof of Theorem 9(ii) it follows that $\delta(G) = 2$. Equations (5) and (6) yield $N_2 = n - 4$ and $N_3 = 4$. Thus, we have

$$\widetilde{Lz}(G) = 4(2n - 5) < \widetilde{Lz}(G^\star) = \begin{cases} 35 & \text{if } n = 6, \\ 48 & \text{if } n = 7, \end{cases}.$$

a contradiction, where $G^\star$ is the n-order connected tricyclic graph with maximum degree $n - 1$ and minimum degree at least 2 (see Figure 11). □

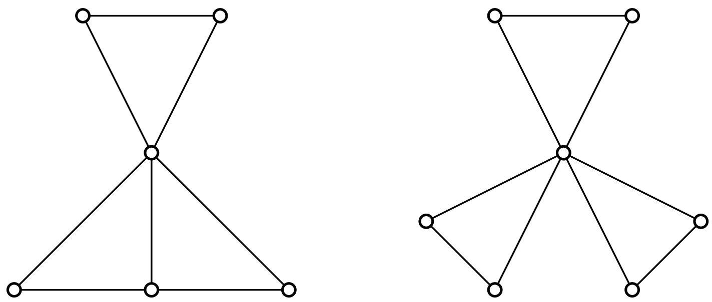

Figure 11. The n-order connected tricyclic graphs $G^\star$ of maximum degree $n - 1$ and minimum degree no less than 2, for $n = 6, 7$.

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4. Extremal Results Concerning Molecular ξ-Cyclic Graphs

Note that the extremal graphs specified in Theorems 9, 10 and 11 are molecular ones, except for $n = 6, 7$, in Theorem 11. Thus, these graphs remain extremal if one puts the following additional constraint on the graphs considered in these theorems: maximum degree is at most 4. Also, from the proof of Theorem 11 we deduce that the graphs with $(\Delta, \delta) = (3, 2)$ are the only graphs possessing the highest ad-hoc Lanzhou index in the set of all n-order molecular connected tricyclic graphs for $n = 6, 7$. Next, we turn our attention to the results concerning the minimum ad-hoc Lanzhou index of molecular (n, m)-graphs (or, equivalently n-order ξ-cyclic graphs). An (n, m)-graph is an n-order graph of size m. For a graph G, define

$$H_f(G) = \sum_{s \in V(G)} f(d_s). \tag{7}$$

where f is a real-valued function. Some initial studies, recent developments, and a survey on the indices of the form (7) can be found in [21,22], [23–25,27], and [26], respectively.

Lemma 13. [28] *Consider a molecular (n, m)-graph G, where $n \geq 5$. Take*

$$\psi_1 = -\frac{2}{3}f(1) + f(2) - \frac{1}{3}f(4) \quad \text{and} \quad \psi_2 = -\frac{1}{3}f(1) + f(3) - \frac{2}{3}f(4).$$

If $\min\{\psi_1, \psi_2\} > 0$ and $\psi_2/2 < \psi_1 < 2\psi_2$, then

$$H_f(G) \geq \frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m$$

$$+ \begin{cases} f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4) & \text{if } 2m - n \equiv 1 \pmod 3 \\ f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4) & \text{if } 2m - n \equiv 2 \pmod 3 \\ 0 & \text{if } 2m - n \equiv 0 \pmod 3 \end{cases}$$

where the equality holds if and only if the degree set of G is
- *$\{1, 2, 4\}$ and G admits exactly one vertex of degree 2 whenever $2m - n \equiv 1 \pmod 3$;*
- *$\{1, 3, 4\}$ and G admits exactly one vertex of degree 3 whenever $2m - n \equiv 2 \pmod 3$;*
- *$\{1, 4\}$ whenever $2m - n \equiv 0 \pmod 3$.*

Theorem 12. *For a molecular (n, m)-graph G, with $n \geq 8$, the following holds:*

$$\widetilde{Lz}(G) \geq 2m(n-8)(n-4) + 4n(2n-7)$$

$$+ \begin{cases} 2(2n-9) & \text{if } 2m - n \equiv 1 \pmod 3 \\ 4(n-5) & \text{if } 2m - n \equiv 2 \pmod 3 \\ 0 & \text{if } 2m - n \equiv 0 \pmod 3 \end{cases}$$

where the equality characterization is the same as mentioned in Lemma 13.

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Proof. Consider $f(x) = x(n-1-x)^2$ with $n \geq 8$. Then, we have

$$-\frac{2}{3}f(1) + f(2) - \frac{1}{3}f(4) > 0,$$

$$-\frac{1}{3}f(1) + f(3) - \frac{2}{3}f(4) > 0,$$

and

$$\frac{1}{2}\Big(-\frac{1}{3}f(1) + f(3) - \frac{2}{3}f(4)\Big) < -\frac{2}{3}f(1) + f(2) - \frac{1}{3}f(4) < 2\Big(-\frac{1}{3}f(1) + f(3) - \frac{2}{3}f(4)\Big).$$

Thus, by Lemma 13, the desired result follows. □

One of the simple but noticeable consequences of Theorem 12 is the following extremal result involving molecular trees.

Corollary 3. *For every $n \geq 8$, in the family of all n-order molecular trees, only the trees having the degree set*

(i) $\{1,2,4\}$ *and admitting exactly one vertex of degree 2, possess the least value of $\widetilde{Lz}$, when $n \equiv 0 \pmod 3$;*
(ii) $\{1,3,4\}$ *and admitting exactly one vertex of degree 3, possess the least value of $\widetilde{Lz}$, when $n \equiv 1 \pmod 3$;*
(iii) $\{1,4\}$ *possess the least value of $\widetilde{Lz}$, when $n \equiv 2 \pmod 3$.*

5. Extremal Results for n-Order Graphs

To prove the first extremal result involving $\widetilde{Lz}$ for n-order graphs, we require the following known result:

Lemma 14. [10] *If G is an n-order graph, then*

$$0 \leq Lz(G) \leq \frac{4n(n-1)^3}{27}.$$

Here the left equality is true if and only if $G \in \{K_n, \overline{K}_n\}$, and the right equality is true if and only if $n \equiv 1$ (mod 3) and G is a $\frac{2(n-1)}{3}$ - regular graph.

Proposition 3. *In the set of all n-order graphs, only the edgeless graph $\overline{K}_n$ and the complete graph K_n possess the least value of $\widetilde{Lz}$; the mentioned least value is 0. Also, in the same set with the constraint $n \equiv 1 \pmod 3$, only the $\frac{(n-1)}{3}$-regular graph possesses the highest value of $\widetilde{Lz}$; the mentioned highest value is*

$$\frac{4n(n-1)^3}{27}.$$

Proof. Since $Lz(\overline{G}) = \widetilde{Lz}(G)$, by Lemma 14 it is enough to show the existence of at least one $\frac{(n-1)}{3}$-regular graph with n vertices satisfying the congruence $n \equiv 1 \pmod 3$. Since $n \equiv 1 \pmod 3$, we have $n-1 = 3k$ for some integer k. Thus, if $n-1$ is even then k must be even and thereby $\frac{n-1}{3}$ remains even. Eventually, whether $n-1$ is even or odd, in either case, we conclude that $\frac{n(n-1)}{3}$ is even. Also, it is a well-known observation that there exists at least one t-regular graph with order n whenever tn is even; this fact implies that there exists at least one $\frac{(n-1)}{3}$-regular graph with order n for every n satisfying $n \equiv 1 \pmod 3$.
□

Next, we pay our attention to the extremum values of $\widetilde{Lz}$ for n-order molecular graphs.

Theorem 13. *In the set of all n-order molecular graphs, with the constraint $n \geq 14$, only 4-regular graphs possess the highest value of $\widetilde{Lz}$.*

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Proof. Consider an n-order molecular graph G. For every $s \in V(G)$, it holds that $d_s(n-1-d_s)^2 \leq 4(n-5)^2$ with equality if and only if $d_s = 4$. Consequently, we have

$$\widetilde{Lz}(G) \leq 4n(n-5)^2, \tag{8}$$

where the equality is true if and only if G is 4-regular. Since at least one 4-regular graph exists for every $n \geq 14$, the desired result follows from (8). □

For the minimal version of Theorem 13, we require the following:

Lemma 15. *If G is an n-order molecular graph, with $n \geq 14$, and $st \in E(G)$, then*

$$\widetilde{Lz}(G) > \widetilde{Lz}(G - st).$$

Proof. Since the function $f(x) = x(n-1-x)^2$, with $n \geq 14$, is strictly increasing for $x \geq 0$, we get

$$\widetilde{Lz}(G) - \widetilde{Lz}(G - st) = d_s(n-1-d_s)^2 + d_t(n-1-d_t)^2$$
$$- (d_s - 1)(n-2-d_s)^2 + (d_t - 1)(n-2-d_t)^2 > 0,$$

where $d_s = d_s(G)$ and $d_t = d_t(G)$. □

Theorem 14. *For every $n \geq 14$, in the set of all n-order connected molecular graphs, only the trees having the degree set*

(i) $\{1,2,4\}$ *and admitting exactly one vertex of degree* 2*, possess the least value of* $\widetilde{Lz}$*, when* $n \equiv 0 \pmod 3$*;*
(ii) $\{1,3,4\}$ *and admitting exactly one vertex of degree* 3*, possess the least value of* $\widetilde{Lz}$*, when* $n \equiv 1 \pmod 3$*;*
(iii) $\{1,4\}$ *possess the least value of* $\widetilde{Lz}$*, when* $n \equiv 2 \pmod 3$*.*

Proof. Consider an n-order connected molecular graph G containing at least one cycle, where $n \geq 14$. By Lemma 15, it holds that $\widetilde{Lz}(G) > \widetilde{Lz}(G - st)$, where st is an edge lying on a cycle of G. Thus, for every $n \geq 14$, a graph possessing the least value of $\widetilde{Lz}$ in the set of all n-order connected molecular graphs must be a tree. Consequently, the desired conclusion follows from Corollary 3. □

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