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Research Article

Lanzhou index of trees and unicyclic graphs

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Abstract

Let G be a simple graph with vertex set $V(G)$. The Lanzhou index of G is defined as $Lz(G) = \sum_{u\in V(G)} d_{\overline{G}}(u)d_G(u)^2$, where $d_G(u)$ denotes the degree of the vertex u in G and $\overline{G}$ is the complement of G. In this paper, we establish an upper bound on the Lanzhou index for trees of order n with maximum degree Δ. Additionally, we obtain the minimum and maximum values of the Lanzhou index for unicyclic graphs of order n. Moreover, we determine the Lanzhou index's maximum value for chemical trees of order n.

Keywords: Lanzhou index; tree; unicyclic graph; extremal value.

2020 Mathematics Subject Classification: 05C05, 05C07, 05C09, 05C35.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $n = |V(G)|$ and $m = |E(G)|$ the number of vertices and edges of G, respectively. For $u \in V(G)$, we denote by $N_G(u)$ the open neighborhood of u in G, which is the set of vertices adjacent to u. The degree $d_G(u)$ (or $d(u)$) of u in G is the cardinality of $N_G(u)$. Denote by $\Delta(G)$ (or Δ) the maximum degree of G. The cardinality of the set $\{u \in V(G) \mid d(u) = t\}$ is denoted by $n_t(G)$ (or n_t). The complement of G is denoted by $\overline{G}$. The edge connecting the vertices u and v is denoted by uv. For the terminologies and notations not defined here, we refer the readers to [3].

Many degree-based topological indices have been defined in the mathematical-chemical literature. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ belong to the family of the most studied degree-based topological indices. These indices are defined [8–10, 13] as

$$M_1(G) = \sum_{uv\in E(G)} (d(u) + d(v)) = \sum_{v\in V(G)} d^2(v) \quad \text{and} \quad M_2(G) = \sum_{uv\in E(G)} d(u)d(v).$$

The forgotten index is another well-known degree-based topological index. It is defined [6] for G as

$$F(G) = \sum_{u\in V(G)} = d^3(u).$$

Recently, De et al. [4] and Khaksari et al. [11], Vukicević et al. [14], independently proposed and investigated the following degree-based topological index, which is known as the Lanzhou index and also the forgotten coindex:

$$Lz(G) = \sum_{u\in V(G)} d_{\overline{G}}(u)d_G(u)^2 = (n-1)M_1(G) - F(G).$$

In [14], it was shown that the Lanzhou index behaves better than several existing indices of this kind in predicting a chemically relevant property of nonane isomers, and some mathematical results concerning extremal structures were established. In [5], Liu et al. established a best possible lower bound for the Lanzhou index of trees in terms of their order and degree, and they characterized all extremal trees. In [15], Wang and Mao studied the Lanzhou index of several classes of hexagonal systems, obtained the Lanzhou index of trees with given diameters, investigated this index for Cartesian product graphs, and found Nordhaus-Gaddum-type results. Additional mathematical properties of the Lanzhou index can be found in [1, 2, 7, 12].

In this paper, we obtain an upper bound on the Lanzhou index for trees of order n with maximum degree Δ, and characterize the corresponding extremal graphs. Additionally, we obtain the extremum values of the Lanzhou index for unicyclic graphs of order n. Besides that, we determine the Lanzhou index's maximum value for chemical trees of order n.

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2. The maximum value of Lanzhou index of trees with given maximum degree

Let T_n^Δ be the set of trees on n vertices with the maximum degree Δ. Then $\bigcup_{\Delta\le 4} T_n^\Delta$ is the set of all chemical trees with n vertices. We first introduce a transformation.

Transformation 2.1. *Let $T \in T_n^\Delta$ and $u, v \in V(T)$ with $1 < d_T(v) \le d_T(u) < \Delta$. Take $w \in N_G(v) \setminus N_G(u)$. Denote by T' the tree obtained from T by deleting edge vw and adding edge uw. Then $T' \in T_n^\Delta$, $d_{T'}(u) = d_T(u) + 1$, $d_{T'}(v) = d_T(v) - 1$, and $d_T(x) = d_{T'}(x)$ for all $x \in V(T) \setminus \{u, v\}$.*

Theorem 2.1. *Let $T \in T_n^\Delta$.*

(I). *For $2 \le \Delta < \frac{n+2}{3}$ and $n \equiv i + 1 \pmod{\Delta - 1}$, where $1 \le i \le \Delta - 1$,*

$$Lz(T) \le \frac{(-n+1+i)\Delta^3 + (n-1)(n-1-i)\Delta^2 + (n^2+ni^2-i^2-i^3-3n+2)\Delta - (n-1-i)(i^2+n-2) - (n-2)(n-1)}{\Delta - 1}$$

with equality if and only if the degree sequence of T is

$$\overbrace{\Delta, \cdots, \Delta}^{\frac{n-1-i}{\Delta-1}}, i, \overbrace{1, \cdots, 1}^{n-\frac{n-1-i}{\Delta-1}-1}.$$

(II). *Let $\frac{n+2}{3} \le \Delta \le \frac{n+5}{3}$.*

(i). *If $n \equiv 0 \pmod 3$, then*

$$Lz(T) \le -3\Delta^2 + (3n+3)\Delta^2 - (4n+2)\Delta + n^2 - 3n + 6$$

with equality if and only if the degree sequence of T is $\Delta, \Delta-1, \Delta-1, \overbrace{1, \cdots, 1}^{n-3}$.

(ii). *If $n \equiv 1 \pmod 3$ and $\Delta = \frac{n+2}{3} (n \ne 7)$, then*

$$Lz(T) \le -3\Delta^3 + 3n\Delta^2 - (2n+1)\Delta + n^2 - 4n + 6$$

with equality if and only if the degree sequence of T is $\Delta, \Delta, \Delta-1, \overbrace{1, \cdots, 1}^{n-3}$. If $n = 7$, then $Lz(T) \le 90$ with equality if and only if the degree sequence of T is $3, 3, 2, 1, 1, 1, 1$ or $3, 2, 2, 2, 1, 1, 1$.

(iii). *If $n \equiv 1 \pmod 3$ and $\Delta = \frac{n+5}{3}$, then*

$$Lz(T) \le -3\Delta^3 + (3n+9)\Delta^2 - (8n+40)\Delta + n^2 + 11n + 54$$

with equality if and only if the degree sequence of T is $\Delta, \Delta, \Delta-4, \overbrace{1, \cdots, 1}^{n-3}$ or $\Delta, \Delta-1, \Delta-3, \overbrace{1, \cdots, 1}^{n-3}$ or $\Delta, \Delta-2, \Delta-2, \overbrace{1, \cdots, 1}^{n-3}$.

(iv). *If $n \equiv 2 \pmod 3$, then*

$$Lz(T) \le -3\Delta^3 + (3n+6)\Delta^2 - (6n+9)\Delta + n^2 + 10$$

with equality if and only if the degree sequence of T is $\Delta, \Delta-1, \Delta-2, \overbrace{1, \cdots, 1}^{n-3}$.

(III). *If $\frac{n+5}{3} < \Delta \le \frac{n}{2}$, then*

$$Lz(T) \le 6\Delta^3 - 6(n+3)\Delta^2 + 2(n^2+6n+5)\Delta - n^2 - 9n + 4$$

with equality if and only if the degree sequence of T is $\Delta, \Delta, n+1-2\Delta, \overbrace{1, \cdots, 1}^{n-3}$.

(IV). *If $\frac{n+1}{2} \le \Delta \le n-1$, then*

$$Lz(T) \le -(n+2)\Delta^2 + (n^2+2n)\Delta - 4n + 4$$

with equality if and only if the degree sequence of T is $\Delta, n-\Delta, \overbrace{1, \cdots, 1}^{n-2}$.

Proof. Let $T \in T_n^{\Delta}$ be a tree with the maximum Lanzhou index. If there are two vertices u, v in T such that $1 < d(v) \leq d(u) < \Delta$, we choose such vertices with the assumption that $d(u) + d(v)$ is as small as possible. Let $d(v) = i$ and $d(u) = j$ and T_1 be the tree obtained from T by applying Transformation 2.1, then

$$\begin{aligned}
Lz(T_1) - Lz(T) &= \sum_{w \in V(T_1)} d_{\overline{T_1}}(w) d_{T_1}(w)^2 - \sum_{w \in V(T)} d_{\overline{T}}(w) d_T(w)^2 \\
&= (j+1)^2(n-1-j-1) + (i-1)^2(n-1-i+1) - i^2(n-1-i) - j^2(n-1-j) \\
&= (n-1-j)(2j+1) - (n-1-i)(2i-1) + (i-1)^2 - (j+1)^2 \\
&= 2nj - 2j - 2j^2 + n - 1 - j - (2ni - 2i - 2i^2 - n + 1 + i) + (i-1)^2 - (j+1)^2 \\
&= 2n(j-i) - 2(j-i) - 2(j^2 - i^2) + 2n - 2 - (i+j) + i^2 - 2i + 1 - j^2 - 2j - 1 \\
&= (2n-2)(j-i) + 3(i^2 - j^2) - 3(i+j) + 2n - 2 \\
&= (j-i)(2n - 2 - 3(i+j)) + 2n - 2 - 3(i+j) \\
&= (j-i+1)(2n-2-3(i+j)),
\end{aligned}$$

i.e.,

$$Lz(T_1) - Lz(T) = (j-i+1)(2n-2-3(i+j)) = (j-i+1)\alpha \tag{1}$$

where $j - i + 1 > 0$ and $\alpha = 2n - 2 - 3(i+j)$.

Case 1. $2 \leq \Delta < \frac{n+2}{3}$.
In this case, we have

$$\alpha = 2n - 2 - 3(i+j) \geq 2n - 2 - 3(2\Delta - 2) = 2n + 4 - 6\Delta > 2n + 4 - \frac{6(n+2)}{3} = 0$$

and thus $Lz(T_1) > Lz(T)$, which is a contradiction. Hence, there are no two vertices u, v in T such that $1 < d_T(v) \leq d_T(u) < \Delta$. So, $\sum_{t=2}^{\Delta-1} n_t(T) \leq 1$.

Subcase 1.1. If $\sum_{t=2}^{\Delta-1} n_t(T) = 0$, then

$$\begin{cases} n = n_1 + n_{\Delta} \\ 2n - 2 = \Delta n_{\Delta} + n_1 \end{cases}$$

and $n_{\Delta} = \frac{n-2}{\Delta-1}$. Therefore, $n \equiv 2 \pmod{\Delta - 1}$, the degree sequence of T is $\overbrace{\Delta, \cdots, \Delta}^{\frac{n-2}{\Delta-1}}, \overbrace{1, \cdots, 1}^{n-\frac{n-2}{\Delta-1}}$, and

$$Lz(T) = \frac{n-2}{\Delta-1}\Delta^2(n-1-\Delta) + (n - \frac{n-2}{\Delta-1})(n-2) = \frac{(n-2)(n\Delta^2 - \Delta^2 - \Delta^3 + n\Delta - 2n + 2)}{\Delta - 1}.$$

Subcase 1.2. If $\sum_{t=2}^{\Delta-1} n_t(T) = 1$, let v be the unique vertex in T with $1 < d_T(v) = i < \Delta$, then

$$\begin{cases} n = n_1 + n_i + n_{\Delta} = n_1 + 1 + n_{\Delta} \\ 2n - 2 = \Delta n_{\Delta} + n_1 + i \end{cases}$$

and $n_{\Delta} = \frac{n-i-1}{\Delta-1}$. Hence $n \equiv i + 1 \pmod{\Delta - 1}$, the degree sequence of T is $\overbrace{\Delta, \cdots, \Delta}^{\frac{n-1-i}{\Delta-1}}, i, \overbrace{1, \cdots, 1}^{n-\frac{n-1-i}{\Delta-1}-1}$, and

$$\begin{aligned}
Lz(T) &= n_{\Delta}\Delta^2(n-1-\Delta) + i^2(n-1-i) + (n - 1 - \frac{n-i-1}{\Delta-1})(n-2) \\
&= \frac{(-n+1+i)\Delta^3 + (n-1)(n-1-i)\Delta^2 + (n^2 + ni^2 - i^2 - i^3 - 3n + 2)\Delta - (n-1-i)(i^2+n-2) - (n-2)(n-1)}{\Delta - 1}.
\end{aligned}$$

In summary, if $2 \leq \Delta < \frac{n+2}{3}$ and $n \equiv i + 1 \pmod{\Delta - 1}$, where $1 \leq i \leq \Delta - 1$, then

$$Lz(T) \leq \frac{(-n+1+i)\Delta^3 + (n-1)(n-1-i)\Delta^2 + (n^2 + ni^2 - i^2 - i^3 - 3n + 2)\Delta - (n-1-i)(i^2+n-2) - (n-2)(n-1)}{\Delta - 1}$$

with equality if and only if the degree sequence of T is

$$\overbrace{\Delta, \cdots, \Delta}^{\frac{n-1-i}{\Delta-1}}, i, \overbrace{1, \cdots, 1}^{n-\frac{n-1-i}{\Delta-1}-1}.$$

Case 2. $\Delta > \frac{n+5}{3}$.
Note that $2n-2 = \sum_{w\in V(T)} d(w) \geq i+j+\Delta+(n-3)$, we have $i+j \leq n+1-\Delta$ and $\alpha \geq 2n-2-3(n+1-\Delta) = 3\Delta-n-5 > 0$. Hence, $Lz(T_1) - Lz(T) > 0$, a contradiction. So, there are no two vertices u, v in T such that $1 < d_T(v) \leq d_T(u) < \Delta$. Therefore, $\sum_{t=2}^{\Delta-1} n_t(T) \leq 1$.

Subcase 2.1. If $\sum_{t=2}^{\Delta-1} n_t(T) = 0$, then by the similar arguments provided the proof of Subcase 1.1, we conclude that the degree sequence of T is

$$\overbrace{\Delta,\cdots,\Delta}^{\frac{n-2}{\Delta-1}},\overbrace{1,\cdots,1}^{n-\frac{n-2}{\Delta-1}}$$

and $n \equiv 2 \pmod{\Delta-1}$. Moreover, if $\frac{n+5}{3} < \Delta \leq \frac{n}{2}$, we have $\frac{n-2}{\Delta-1} = 2$. So, the degree sequence of T is $\Delta,\Delta,\overbrace{1,\cdots,1}^{n-2}$ and

$$Lz(T) = -2\Delta^3 + 2(n-1)\Delta^2 + n^2 - 4n + 4.$$

If $\frac{n}{2} < \Delta \leq n-1$, we have $\frac{n-2}{\Delta-1} = 1$. So, the degree sequence of T is $\Delta,\overbrace{1,\cdots,1}^{n-1}$ and $Lz(T) = -\Delta^3 + (n-1)\Delta^2 + n^2 - 3n + 2$.

Subcase 2.2. If $\sum_{t=2}^{\Delta-1} n_t(T) = 1$, let v be the unique vertex in T with $1 < d_T(v) = i < \Delta$, then by the similar arguments given in the proof of Subcase 1.2, we conclude that the degree sequence of T is

$$\overbrace{\Delta,\cdots,\Delta}^{\frac{n-1-i}{\Delta-1}},i,\overbrace{1,\cdots,1}^{n-\frac{n-1-i}{\Delta-1}-1},$$

where $n \equiv i+1 \pmod{\Delta-1}$. Moreover, if $\frac{n+5}{3} < \Delta \leq \frac{n}{2}$, we have $i = n+1-2\Delta$ and $\frac{n-1-i}{\Delta-1} = 2$. So the degree sequence of T is

$$\Delta,\Delta,n+1-2\Delta,\overbrace{1,\cdots,1}^{n-3}$$

and $Lz(T) = 6\Delta^3 - 6(n+3)\Delta^2 + 2(n^2+6n+5)\Delta - n^2 - 9n + 4$. If $\frac{n+1}{2} \leq \Delta \leq n-1$, we have $\frac{n-1-i}{\Delta-1} = 1$ and $i = n-\Delta$. So the degree sequence of T is

$$\Delta,n-\Delta,\overbrace{1,\cdots,1}^{n-2}$$

and $Lz(T) = -(n+2)\Delta^2 + (n^2+2n)\Delta - 4n + 4$.

In summary, if $\frac{n+5}{3} < \Delta \leq \frac{n}{2}$, then $Lz(T) \leq 6\Delta^3 - 6(n+3)\Delta^2 + 2(n^2+6n+5)\Delta - n^2 - 9n + 4$ with equality if and only if the degree sequence of T is

$$\Delta,\Delta,n+1-2\Delta,\overbrace{1,\cdots,1}^{n-3},$$

while if $\frac{n+1}{2} \leq \Delta \leq n-1$, then $Lz(T) \leq -(n+2)\Delta^2 + (n^2+2n)\Delta - 4n + 4$ with equality if and only if the degree sequence of T is

$$\Delta,n-\Delta,\overbrace{1,\cdots,1}^{n-2}.$$

Case 3. $\frac{n+2}{3} \leq \Delta \leq \frac{n+5}{3}$.
Let $n = 3q + r$, where $r \in \{0,1,2\}$. Then $q + \frac{r+2}{3} \leq \Delta \leq q + \frac{r+5}{3}$.

Subcase 3.1. If $r = 0$, i.e., $n = 3q$, then $q + \frac{2}{3} \leq \Delta \leq q + \frac{5}{3}$ and $\Delta = q+1$. Since $2n-2 = \sum_{w\in V(T)} d(w) \geq i+j+\Delta+(n-3)$, we have $i+j \leq 2\Delta - 2$ with equality if and only if the degree sequence of T is

$$\Delta,\Delta-1,\Delta-1,\overbrace{1,\cdots,1}^{n-3}.$$

Subcase 3.1.1. If $i+j \leq 2\Delta-3$, then $\alpha = 2n-2-3(i+j) \geq 2n-2-3(2\Delta-3) = 6q-2-3(2q-1) = 1 > 0$, and $Lz(T_1) - Lz(T) > 0$, a contradiction. Hence, there is at most one vertex v in T such that $1 < d_T(v) < \Delta$. Thus, $\sum_{t=2}^{\Delta-1} n_t \leq 1$. If $\sum_{t=2}^{\Delta-1} n_t = 0$, then

$$\begin{cases} n_1 + n_\Delta = n \\ \Delta n_\Delta + n_1 = 2n-2 \end{cases}$$

and we have $n_\Delta = 3 - \frac{2}{q}$ from $n = 3q$ and $\Delta = q+1$. Since n_Δ is a positive integer, it must be $q = 2$ or $q = 1$. If $q = 2$, we have $\Delta = q+1 = 3$, $n_\Delta = 2$, $n = 6$, and the degree sequence of T is $3,3,1,1,1,1$. So,

$$Lz(T) = 2\times 3^2(5-3) + 4(5-1) = 52 \leq Lz(T^*) = 54,$$

where the degree sequence of T^* is $3, 2, 2, 1, 1, 1$. If $q = 1$, we have $\Delta = 2$, $n_\Delta = 1$, $n = 3$, and the degree sequence of T is $2, 1, 1$. So, $Lz(T) = 2$.
If $\sum_{t=2}^{\Delta-1} n_t = 1$, then

$$\begin{cases} n_1 + n_\Delta + n_i = n = 3q \\ \Delta n_\Delta + n_1 + i = 2n - 2 = 6q - 2 \end{cases}$$

and we have $n_\Delta = 3 - \frac{1+i}{q}$ from $n_i = 1$ and $n = 3q$ and $\Delta = q + 1$. Since n_Δ is a positive integer and $2 \leq i \leq \Delta - 2$, we have $i = q - 1$ and $n_\Delta = 2$. The degree sequence of T is

$$\Delta, \Delta, \Delta - 2, \overbrace{1, \cdots, 1}^{n-3},$$

and $Lz(T) = -3\Delta^3 + (3n + 3)\Delta^2 - 4(n + 2)\Delta + n^2 - n + 10 < -3\Delta^3 + (3n + 3)\Delta^2 - 2(2n + 1)\Delta + n^2 - 3n + 6$.

Subcase 3.1.2. If $i+j > 2\Delta-3$, then $i = j = \Delta-1$ from $2 \leq i \leq j \leq \Delta-1$. Note that $2n-2 = \sum_{w\in V(T)} d(w) \geq i+j+\Delta+(n-3)$, we have $i + j \leq 2\Delta - 2$ with equality if and only if the degree sequence of T is

$$\Delta, \Delta - 1, \Delta - 1, \overbrace{1, \cdots, 1}^{n-3}.$$

Then $Lz(T) = -3\Delta^3 + (3n + 3)\Delta^2 - 2(2n + 1)\Delta + n^2 - 3n + 6$.

Subcase 3.2. If $r = 1$, i.e., $n = 3q + 1$, then $q + 1 \leq \Delta \leq q + 2$. Note that $2 \leq i \leq j \leq \Delta - 1$, we have $i + j \leq 2\Delta - 2$.

Subcase 3.2.1. $\Delta = q + 1$, i.e., $\Delta = \frac{n+5}{3}$.

Subcase 3.2.1.1. If $i + j < 2\Delta - 2$, then $\alpha = 2n - 2 - 3(i + j) > 2n - 2 - 3(2\Delta - 2) > 6q - 6q = 0$ and $Lz(T_1) - Lz(T) > 0$, a contradiction. Hence, there is at most one vertex v in T such that $1 < d_T(v) < \Delta$, i.e., $\sum_{t=2}^{\Delta-1} n_t \leq 1$. If $\sum_{t=2}^{\Delta-1} n_t = 0$, by

$$\begin{cases} n = n_1 + n_\Delta \\ 2n - 2 = \Delta n_\Delta + n_1 \end{cases}$$

we have $n_\Delta = 3 - \frac{1}{q}$ and $q = 1$ since n_Δ is a positive integer. Then $n = 4$, the degree sequence is $2, 2, 1, 1$, and $Lz(T) = 12$.
If $\sum_{t=2}^{\Delta-1} n_t = 1$, then by

$$\begin{cases} n = n_1 + n_\Delta + n_i = n_1 + n_\Delta + 1 \\ 2n - 2 = \Delta n_\Delta + n_1 + i \end{cases}$$

we have $n_\Delta = 3 - \frac{i}{q}$. Since $2 \leq i \leq \Delta - 1 = q$ and n_Δ is a positive integer, $i = q$, and $n_\Delta = 2$. Then the degree sequence of T is

$$\Delta, \Delta, \Delta - 1, \overbrace{1, \cdots, 1}^{n-3}$$

and $Lz(T) = -3\Delta^3 + 3n\Delta^2 - (2n + 1)\Delta + n^2 - 4n + 6$.

Subcase 3.2.1.2. If $i + j = 2\Delta - 2$, then $i = j = \Delta - 1$ and $n_{\Delta-1} \geq 2$. Also, $n_2 = \cdots = n_{\Delta-2} = 0$ by the minimization of $i + j = d(u) + d(v)$. We have

$$\begin{cases} n = n_1 + n_\Delta + n_{\Delta-1} \\ 2n - 2 = \Delta n_\Delta + n_1 + (\Delta - 1)n_{\Delta-1}. \end{cases}$$

So, $n_\Delta \leq 1 + \frac{1}{q}$ and $n_\Delta \in \{1, 2\}$ since n_Δ is a positive integer. However, if $n_\Delta = 2$, then $q = 1$ and $\Delta = q + 1 = 2$. We have $2 \leq i = j = \Delta - 1 = 1$, a contradiction. So, $n_\Delta = 1$. Now, if there is a vertex $w \in V(T) \setminus \{u, v\}$ such that $1 < d(w) < \Delta$, then

$$\begin{aligned} 2n - 2 &\geq \Delta + 2(\Delta - 1) + d(w) + (n - 4) \\ &\geq 3\Delta + n - 4 \quad (\text{since } \ d(w) \geq 2) \\ i.e., \ \ n &\geq 3\Delta - 2 \\ 3q + 1 &\geq 3(q + 1) - 2 = 3q + 1. \end{aligned}$$

Thus, equality holds in all the above inequalities, which implies that $d(w) = 2$. Also, $d(w) = \Delta - 1$ by the minimization of $i + j = d(u) + d(v)$ again, and thus $\Delta = 3$, $q = 2$, $n = 7$. The degree sequence of T is

$$\Delta, \Delta - 1, \Delta - 1, 2, \overbrace{1, \cdots, 1}^{n-4},$$

i.e., $3, 2, 2, 2, 1, 1, 1$ and $Lz(T) = 90 = Lz(T^*)$ where the degree sequence of T^* is $3, 3, 2, 1, 1, 1, 1$.

Subcase 3.2.2. $\Delta = q+2$, i.e., $\Delta = \frac{n+5}{3}$.
From $2n-2 = \sum_{w\in V(T)} d(w) \geq i+j+\Delta+(n-3)$ and $n = 3q+1 = 3\Delta-5$, we have $i+j \leq 2\Delta-4$.

Subcase 3.2.2.1. If $i+j \leq 2\Delta-5$, then $\alpha = 2n-2-3(i+j) \geq 2n-2-3(2\Delta-5) > 2(3q+1)-2-3(2q-1) = 3 > 0$, and $Lz(T_1)-Lz(T) > 0$, a contradiction. Hence, there is at most one vertex v in T such that $1 < d_T(v) < \Delta$. Thus, $\sum_{t=2}^{\Delta-1} n_t \leq 1$.
If $\sum_{t=2}^{\Delta-1} n_t = 0$, then

$$\begin{cases} n = n_1 + n_\Delta \\ 2n-2 = \Delta n_\Delta + n_1 \end{cases}$$

and $n_\Delta = 3 - \frac{4}{q+1}$. We have $q = 1$ or $q = 3$ since n_Δ is a positive integer. Hence, the degree sequence of T is $3,1,1,1$ or $5,5,1,1,1,1,1,1,1,1$, and $Lz(T) = 6$ or $Lz(T) = 264$, respectively.
If $\sum_{t=2}^{\Delta-1} n_t = 1$, then

$$\begin{cases} n = n_1 + n_\Delta + n_i \\ 2n-2 = \Delta n_\Delta + n_1 + i \end{cases}$$

and $n_\Delta = 3 - \frac{i+3}{q+1} \in \{1,2\}$ since n_Δ is a positive integer.
When $n_\Delta = 1$, we have $i+3 = 2(q+1)$, and $i = 2q-1 \leq \Delta-1 = q+1$. So, $q \leq 2$. If $q = 1$, then $2 \leq i = 2q-1 = 1$, a contradiction. If $q = 2$, then $n = 3q+1 = 7$, $i = 2q-1 = 3$ and the degree sequence of T is

$$\Delta, \Delta-1, \overbrace{1,\cdots,1}^{n-2},$$

i.e., $4,3,1,1,1,1,1$ and thus $Lz(T) = 84$.

When $n_\Delta = 2$, we have $i+3 = q+1$ and $i = q-2 = \Delta-4$. The degree sequence of T is $\Delta, \Delta, \Delta-4, \overbrace{1,\cdots,1}^{n-3}$ and thus $Lz(T) = -3\Delta^3 + (3n+9)\Delta^2 - (8n+40)\Delta + n^2 + 11n + 54$.

Subcase 3.2.2.2. If $i+j = 2\Delta-4$, then $i = \Delta-1$, $j = \Delta-3$ or $i = j = \Delta-2$. Also, the degree sequence of T is

$$\Delta, j, i, \overbrace{1,\cdots,1}^{n-3}$$

from $2n-2 = \sum_{w\in V(T)} d(w) = i+j+\Delta+(n-3)$, i.e., the degree sequence of T is

$$\Delta, \Delta-1, \Delta-3, \overbrace{1,\cdots,1}^{n-3} \quad \text{or} \quad \Delta, \Delta-2, \Delta-2, \overbrace{1,\cdots,1}^{n-3}.$$

Thus, $Lz(T) = -3\Delta^3 + (3n+9)\Delta^2 - (8n+40)\Delta + n^2 + 11n + 54$.

Subcase 3.3. If $r = 2$, i.e., $n = 3q+2$, then $q + \frac{4}{3} = \frac{n+2}{3} \leq \Delta \leq \frac{n+5}{3} = q + \frac{7}{3}$ and $\Delta = q+2$ since Δ is a positive integer. From

$$2n-2 = \sum_{w\in V(T)} d(w) \geq i+j+\Delta+(n-3),$$

we have $i+j \leq 2\Delta-3$.

Subcase 3.3.1. If $i+j \leq 2\Delta-4$, then $\alpha = 2n-2-3(i+j) \geq 2n-2-3(2\Delta-4) = 6q+2-6q = 2 > 0$ and $Lz(T_1)-Lz(T) > 0$, a contradiction. Hence, there is at most one vertex v in T such that $1 < d_T(v) < \Delta$, i.e., $\sum_{t=2}^{\Delta-1} n_t \leq 1$.
If $\sum_{t=2}^{\Delta-1} n_t = 0$, then

$$\begin{cases} n = n_1 + n_\Delta \\ 2n-2 = \Delta n_\Delta + n_1 \end{cases},$$

and $n_\Delta = 3 - \frac{3}{q+1}$. We have $q = 2$ since n_Δ is a positive integer, $n = 3q+2 = 8$, $\Delta = q+2 = 4$. The degree sequence is $4,4,1,1,1,1,1,1$ and thus $Lz(T) = 132 < Lz(T^*) = 134$ where the degree sequence of T^* is $4,3,2,1,1,1,1,1$.
If $\sum_{t=2}^{\Delta-1} n_t = 1$, then

$$\begin{cases} n = n_1 + n_\Delta + n_i = n_1 + n_\Delta + 1 \\ 2n-2 = \Delta n_\Delta + n_1 + i \end{cases}$$

and $n_\Delta = 3 - \frac{2+i}{q+1}$. Because n_Δ is a positive integer, we have either (1) $n_\Delta = 2$, $i = q-1 = \Delta-3$, the degree sequence of T is

$$\Delta, \Delta, \Delta-3, \overbrace{1,\cdots,1}^{n-3}$$

and $Lz(T) = -3\Delta^3 + (3n+6)\Delta^2 - (6n+21)\Delta + n^2 + 4n + 24 < -3\Delta^3 + (3n+6)\Delta^2 - (6n+9)\Delta + n^2 + 10$, or (2) $n_\Delta = 1$, $i = 2q$; note that $2 \le i = 2q = 2(\Delta - 2) \le \Delta - 1$, $\Delta \le 3$ and $q = 1$, $n = 5$, the degree sequence of T is

$$\Delta, \Delta - 1, \overbrace{1, \cdots, 1}^{n-2},$$

i.e., $3, 2, 1, 1, 1$ and thus $Lz(T) = 26$.

Subcase 3.3.2. If $i + j = 2\Delta - 3$, then $i = \Delta - 2$, $j = \Delta - 1$ and $n_{\Delta-1} \ge 1$, $n_{\Delta-2} \ge 1$. From the minimization of $i + j = d(u) + d(v)$, $n_2 = \cdots = n_{\Delta-3} = 0$ and

$$\begin{cases} n = n_1 + n_\Delta + n_{\Delta-1} + n_{\Delta-2} \\ 2n - 2 = n_1 + \Delta n_\Delta + (\Delta-1)n_{\Delta-1} + (\Delta-2)n_{\Delta-2} \end{cases}$$

we have $n - 2 = (\Delta-1)n_\Delta + (\Delta-2)n_{\Delta-1} + (\Delta-3)n_{\Delta-2} \ge (\Delta-1)n_\Delta + 2\Delta - 5$, which gives

$$\begin{aligned} (\Delta-1)n_\Delta &\le n - 2 - 2\Delta + 5 \\ (q+1)n_\Delta &\le 3q - 2(q+2) + 5 = q + 1, \end{aligned}$$

and thus $n_\Delta = 1$, and the degree sequence of T is $\Delta, \Delta-1, \Delta-2, \overbrace{1, \cdots, 1}^{n-3}$. Therefore,

$$Lz(T) = -3\Delta^3 + (3n+6)\Delta^2 - (6n+9)\Delta + n^2 + 10.$$

In summary, if $\frac{n+2}{3} \le \Delta \le \frac{n+5}{3}$, then
(i) $Lz(T) \le -3\Delta^2 + (3n+3)\Delta^2 - (4n+2)\Delta + n^2 - 3n + 6$ for $n \equiv 0 \pmod 3$, with equality if and only if the degree sequence of T is

$$\Delta, \Delta-1, \Delta-1, \overbrace{1, \cdots, 1}^{n-3};$$

(ii) $Lz(T) \le -3\Delta^3 + 3n\Delta^2 - (2n+1)\Delta + n^2 - 4n + 6$ for $n \equiv 1 \pmod 3$ $(n \ne 7)$ and $\Delta = \frac{n+2}{3}$ with equality if and only if the degree sequence of T is

$$\Delta, \Delta, \Delta-1, \overbrace{1, \cdots, 1}^{n-3};$$

$Lz(T) = 90$ for $n = 7$ with equality if and only if the degree sequence of T is either $3, 3, 2, 1, 1, 1, 1$ or $3, 2, 2, 2, 1, 1, 1$;
(iii) $Lz(T) \le -3\Delta^3 + (3n+9)\Delta^2 - (8n+40)\Delta + n^2 + 11n + 54$ for $n \equiv 1 \pmod 3$ and $\Delta = \frac{n+5}{2}$ with equality if and only if the degree sequence of T is

$$\Delta, \Delta, \Delta-4, \overbrace{1, \cdots, 1}^{n-3} \quad \text{or} \quad \Delta, \Delta-1, \Delta-3, \overbrace{1, \cdots, 1}^{n-3} \quad \text{or} \quad \Delta, \Delta-2, \Delta-2, \overbrace{1, \cdots, 1}^{n-3};$$

(iv) $Lz(T) \le -3\Delta^3 + (3n+6)\Delta^2 - (6n+9)\Delta + n^2 + 10$ for $n \equiv 2 \pmod 3$ with equality if and only if the degree sequence of T is

$$\Delta, \Delta-1, \Delta-2, \overbrace{1, \cdots, 1}^{n-3}.$$

□

In [14], a lower bound on the Lanzhou index for chemical trees with n vertices was given. By using Theorem 2.1, we get the maximum Lanzhou index of chemical trees on n vertices.

Corollary 2.1. *Let T be a chemical tree with order $n > 10$.*

(i). *If $n \equiv 0 \pmod 3$ then $Lz(T) \le 6n^2 - 40n + 68$, where the equality holds if and only if the degree sequence of T is*

$$\overbrace{4, \ldots 4}^{\frac{n-3}{3}}, 2, \overbrace{1 \ldots 1}^{n-\frac{2n}{3}}.$$

(ii). *If $n \equiv 1 \pmod 3$ then $Lz(T) \le 6n^2 - 40n + 70$, where the equality holds if and only if the degree sequence of T is*

$$\overbrace{4, \ldots 4}^{\frac{n-4}{3}}, 3, \overbrace{1 \ldots 1}^{n-\frac{2n+1}{3}}.$$

(iii). *If* $n \equiv 2 \pmod 3$ *then* $Lz(T) \le 6n^2 - 38n + 52$*, where the equality holds if and only if the degree sequence of* T *is*

$$\overbrace{4,\ldots 4}^{\frac{n-2}{3}},\ \overbrace{1\ldots 1}^{n-\frac{2n+2}{3}}.$$

Proof. Let T be a chemical tree with order $n > 10$, then $\Delta = 4$ or $\Delta = 3$ or $\Delta = 2$ by the definition of chemical trees.

(i) If $\Delta = 4$, then by Theorem 2.1(I) we have

$$Lz(T) \le \frac{-3i^3 + (3n-3)i^2 + (-15n+78)i + 18n^2 - 102n + 84}{3} \quad \text{(where } 1 \le i \le 3)$$

i.e.,

$$Lz(T) \le \begin{cases} 6n^2 - 40n + 68, & n \equiv 0 \pmod 3 \quad (i = 2), \\ 6n^2 - 40n + 70, & n \equiv 1 \pmod 3 \quad (i = 3), \\ 6n^2 - 38n + 52, & n \equiv 2 \pmod 3 \quad (i = 1). \end{cases}$$

(ii) If $\Delta = 3$, then by Theorem 2.1(I) we have

$$Lz(T) \le \frac{-2i^3 + (2n-2)i^2 + (-8n+34)i + 10n^2 - 48n + 38}{2} \quad \text{(where } 1 \le i \le 2)$$

i.e.,

$$Lz(T) \le \begin{cases} 5n^2 - 27n + 34, & n \equiv 0 \pmod 2 \quad (i = 1), \\ 5n^2 - 27n + 41, & n \equiv 1 \pmod 2 \quad (i = 2). \end{cases}$$

(iii) If $\Delta = 2$, then $T \cong P_n$ and $Lz(P_n) = 4n^2 - 18n + 20$.

When $n \equiv 0 \pmod 3$, we have

$$9n^2 - 60n + 68 > 5n^2 - 27n + 34 \quad \text{and} \quad 6n^2 - 40n + 68 > 5n^2 - 28n + 41.$$

When $n \equiv 1 \pmod 3$, we have

$$6n^2 - 40n + 70 > 5n^2 - 27n + 34 \quad \text{and} \quad 6n^2 - 40n + 70 > 5n^2 - 28n + 41.$$

When $n \equiv 2 \pmod 3$ we have

$$6n^2 - 38n + 52 > 5n^2 - 27n + 34 \quad \text{and} \quad 6n^2 - 38n + 52 > 5n^2 - 28n + 41.$$

□

3. Extremum values of Lanzhou index for unicyclic graphs

Let U_n be a unicyclic graph of order n with its unique circuit $C_t = v_1 v_2 \cdots v_t v_1$. For $i = 1, 2, \ldots, t$, let T_i be the component of $G \setminus E(C_t)$ that contains v_i. Let $V(U_n) = R \cup V_2 \cup V_1$, where $R = \{v \in V(U_n) \mid d(v) > 2\}$, $V_2 = \{v \in V(U_n) \mid d(v) = 2\}$, $V_1 = \{v \in V(U_n) \mid d(v) = 1\}$, $|V_2| = l_2$, $|V_1| = l_1$. Denote by $U_{d(v_1),d(v_2),\ldots d(v_t)}$ the unicyclic graph of order n in which every T_i (where $i = 1, 2, \ldots, t$) is a star (see Figure 1).

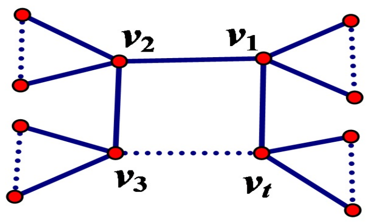

Figure 1: The unicyclic graph $U_{d(v_1),d(v_2),\ldots d(v_t)}$.

Lemma 3.1. *Let* U_n *be a unicyclic graph, then*

$$Lz(U_n) = \sum_{u \in R} \lambda(d_u)(d_u - 1) + l_2 \varphi(2), \tag{2}$$

where $d_u = d(u)$, $\lambda(x) = -x^2 + (n-2)x + 2n - 4$*, and* $\varphi(x) = x^2(n - 1 - x)$.

Proof. Let $\varphi(x) = x^2(n-1-x)$. By the definition of Lanzhou index, we obtain

$$Lz(U_n) = \sum_{u\in V(U_n)} \varphi(d_u) = \sum_{u\in R} \varphi(d_u) + \sum_{u\in V_2} \varphi(d_u) + \sum_{u\in V_1} \varphi(d_u) = \sum_{u\in R} \varphi(d_u) + l_2\varphi(2) + l_1\varphi(1).$$

Since $\sum_{u\in R} d_u + 2l_2 + l_1 = 2n$, we get $\sum_{u\in R}(d_u - 2) = l_1$, which gives

$$\sum_{u\in R}(d_u - 1) = l_1 + |R| = n - l_2. \tag{3}$$

Also, we have

$$\begin{aligned} Lz(U_n) &= \sum_{u\in R} \varphi(d_u) + \sum_{u\in R}(d_u-2)\varphi(1) + l_2\varphi(2) \\ &= \sum_{u\in R}(\varphi(d_u) + (d_u-2)\varphi(1)) + l_2\varphi(2) \\ &= \sum_{u\in R} \frac{\varphi(d_u) + (d_u-2)\varphi(1)}{d_u - 1}(d_u-1) + l_2\varphi(2). \end{aligned}$$

If $\lambda(x) = \frac{\varphi(x)+(x-2)\varphi(1)}{x-1} = -x^2 + (n-2)x + 2n - 4$ then we have

$$Lz(U_n) = \sum_{u\in R} \lambda(x)(d_u - 1) + l_2\varphi(2).$$

$\square$

Lemma 3.2. *Let $U_n (n > 8)$ be a unicyclic graph with its unique circuit $C_t (t \geq 4)$. If U_n has the maximum Lanzhou index, then $l_2 = 0$ or $l_2 = 1$.*

Proof. Let U_n be a unicyclic graph with the maximum Lanzhou index. Suppose there are two vertices u, v in U_n such that $d(u) = d(v) = 2$.

Case 1. $u, v \in V(C_t)$.

Subcase 1.1. $uv \in E(C_t)$. Take $vw \in E(C_t)$ and let U_n^1 be a unicyclic graph obtained from U_n by deleting edge vw and adding edge uw. Then $d_{U_n^1}(u) = 3$, $d_{U_n^1}(v) = 1$ and $d_{U_n^1}(x) = d_{U_n}(x)$ for all $x \in V(U_n)\backslash\{u, v\}$. By the definition of the Lanzhou index, we have

$$\begin{aligned} Lz(U_n^1) - Lz(U_n) &= \sum_{z\in V(U_n^1)} d_{\overline{U_n^1}}(w)d^2_{U_n^1}(w) - \sum_{z\in V(U_n)} d_{\overline{U_n}}(w)d^2_{U_n}(w) \\ &= d^2_{U_n^1}(u)(n-1-d_{U_n^1}(u)) + d^2_{U_n^1}(v)(n-1-d_{U_n^1}(v)) - d^2_{U_n}(u)(n-1-d_{U_n}(u)) - d^2_{U_n}(v)(n-1-d_{U_n}(v)) \\ &= 2n - 16 > 0, \end{aligned}$$

which is a contradiction.

Subcase 1.2. $uv \notin E(C_t)$. Take $vw_1, vw_2 \in E(C_t)$ and let U_n^1 be a unicyclic graph obtained from U_n by deleting edges vw_1, vw_2 and adding edges w_1w_2, uv. Then $d_{U_n^1}(u) = 3$, $d_{U_n^1}(v) = 1$ and $d_{U_n^1}(x) = d_{U_n}(x)$ for all $x \in V(U_n)\backslash\{u, v\}$, which gives a contradiction (the proof is similar to the one provided in Subcase 1.1).

Case 2. $u \in V(C_t)$, $v \in V(U_n)\backslash V(C_t)$ or $u, v \in V(U_n)\backslash V(C_t)$.
Take $vw_1, vw_2 \in E(U_n)$ and let U_n^1 be a unicyclic graph obtained from U_n by deleting edges vw_1, vw_2 and adding edges w_1w_2, uv. Then $d_{U_n^1}(u) = 3$, $d_{U_n^1}(v) = 1$ and $d_{U_n^1}(x) = d_{U_n}(x)$ for all $x \in V(U_n)\backslash\{u, v\}$, which gives a contradiction (the proof is similar to the one provided in Subcase 1.1). $\square$

Lemma 3.3. *Let $U_n (n > 8)$ be a unicyclic graph with its unique circuit C_3. If U_n has the maximum Lanzhou index, then $l_2 = 0$ or $l_2 = 1$.*

Proof. Let U_n be a unicyclic graph with the maximum Lanzhou index. Suppose there are two vertices u, v in U_n such that $d(u) = d(v) = 2$.

Case 1. $u, v \in V(C_3)$. We only need to prove there is at most one vertex $u \in V(C_3)$ with $d(u) = 2$.

Subcase 1.1. $uv \in E(C_3)$.

Subcase 1.1.1. If $U_n \cong U_{2,2,n}$, then $LZ(U_{2,3,n-1}) - Lz(U_{2,2,n}) = 5n - 24 > 0$, which is a contradiction.

Subcase 1.1.2. Suppose that $u, v \in V(C_3)$ and there is a vertex w such that $d(w) = l > 2$ and $w \notin V(C_3)$. Let $w_1, \cdots, w_l$ be the neighbours of w. Let U_n^1 be the unicyclic graph obtained from U_n by deleting edges $ww_3, \ldots, ww_l$ and adding edges $vw_3, \ldots, vw_l$, then $d_{U_n^1}(w) = d_{U_n}(v) = 2$, $d_{U_n^1}(v) = d_{U_n}(w) = l$ and $d_{U_n^1}(x) = d_{U_n}(x)$ for all $x \in V(U_n)\backslash\{w, v\}$. By the definition of the Lanzhou index, we have $Lz(U_n) = Lz(U_n^1)$ and the unique circuit of U_n^1 has at most one vertex of degree 2 (the proof of this fact is similar to the one given in Case 2 of Lemma 3.2). We have $l_2(U_n^1) = 1$ or $l_2(U_n^1) = 0$, and $l_2(U_n) = 1$ or $l_2(U_n) = 0$.

Subcase 1.1.3. Suppose that $u, v \in V(C_3)$ and $\forall\ w \in V(U_n)\backslash V(C_3)$, $d(w) = 2$. Let U_n^2 be the unicyclic graph obtained from U_n by deleting the edge ww_1 and adding the edge vw_1, where $w_1 \notin V(C_3)$, then $d_{U_n^2}(v) = 3$, $d_{U^2}(w) = 1$ and $d_{U_n^1}(x) = d_{U_n}(x)$ for all $x \in V(U_n)\backslash\{w, v\}$. By the definition of the Lanzhou index, we have $Lz(U_n^2) - Lz(U_n) = 2n - 14 > 0$, which is a contradiction.

Case 2. $u \in V(C_3)$, $v \in V(U_n)\backslash V(C_3)$ or $u, v \in V(U_n)\backslash V(C_t)$. The proof is similar to the one given in Case 2 of Lemma 3.2. □

Lemma 3.4. *Let n be an even integer and U_n be a unicyclic graph with n vertices, where $n \geq 25$. If there is no vertex v with $d(v) = 2$ in U_n, then $Lz(U_n) \leq \frac{n^3}{4} + \frac{n^2}{2} + 4n - 30$ with equality if and only if $U_n \cong U_{\frac{n}{2},\frac{n}{2},3}$.*

Proof. By Equation (2), we have

$$\begin{aligned} Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right) &= \lambda\left(\frac{n}{2}\right)\left(\frac{n}{2}-1\right) + \lambda\left(\frac{n}{2}\right)\left(\frac{n}{2}-1\right) + \lambda(3)(3-1) \\ &= \left(\frac{n^2}{4}+n-4\right)\left(\frac{n}{2}-1\right) + \left(\frac{n^2}{4}+n-4\right)\left(\frac{n}{2}-1\right) + 2(5n-19) \\ &= \frac{n^3}{4} + \frac{n^2}{2} + 4n - 30. \end{aligned}$$

Case 1. Suppose that $\Delta < \frac{n}{2} - 1$. Let $u_i \in R$, $d(u_i) = x_i \geq 3$ and $\lambda(x_1) \geq \lambda(x_2) \ldots \geq \lambda(x_k)$. Then, we have

$$\begin{aligned} Lz(U_n) &= \lambda(x_1)(x_1-1) + \lambda(x_2)(x_2-1) + \ldots + \lambda(x_k)(x_k-1) \\ &= \underbrace{\lambda(x_1) + \ldots + \lambda(x_1)}_{x_1-1} + \ldots + \underbrace{\lambda(x_k) + \ldots + \lambda(x_k)}_{x_k-1} \quad \left(\text{as} \sum_{i=1}^{k}(x_i-1) = n\right) \\ &\leq \lambda\left(\frac{n}{2}-2\right)\left(\frac{n}{2}-3\right) + \lambda\left(\frac{n}{2}-2\right)\left(\frac{n}{2}-3\right) + 6\lambda(7) \\ &= \frac{n^3}{4} - \frac{n^2}{2} + 34n - 378 < Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right). \end{aligned}$$

Case 2. Suppose that $\Delta \geq \frac{n}{2} - 1$ and there are at least two vertices of degree greater than or equal to $\frac{n}{2} - 1$.

Claim 1: There are at most two vertices of degree greater than or equal to $\frac{n}{2} - 1$.

Proof of Claim 1. Suppose that there exist $v_1, \cdots, v_l \in R$ $(l \geq 3)$ with $d(v_i) \geq \frac{n}{2} - 1$ for $1 \leq i \leq l$. We have

$$\sum_{i=1}^{l}(x_i - 1) \geq 3\left(\frac{n}{2} - 1 - 1\right) = \frac{3n}{2} - 6 > n,$$

which contradicts Equation (3). So, there are at most two vertices of degree greater than or equal to $\frac{n}{2} - 1$ in U_n.

By Equation (3) and Claim 1, there are following four possibilities about the degree sequence of U_n:

$$\frac{n}{2}, \frac{n}{2}-1, 4, \overbrace{1, 1 \ldots 1}^{n-3}; \qquad \frac{n}{2}-1, \frac{n}{2}-1, 5, \overbrace{1, 1 \cdots 1}^{n-3}; \qquad \frac{n}{2}-1, \frac{n}{2}-1, 3, 3, \overbrace{1, 1 \ldots 1}^{n-4}; \qquad \frac{n}{2}+1, \frac{n}{2}-1, 3, \overbrace{1, 1 \cdots 1}^{n-3}.$$

If the degree sequence of U_n is $\frac{n}{2}, \frac{n}{2}-1, 4, \overbrace{1, 1 \ldots 1}^{n-3}$, then we have

$$\begin{aligned} Lz(U_n) &= \left(\frac{n}{2}\right)^2\left(n-1-\frac{n}{2}\right) + \left(\frac{n}{2}-1\right)^2\left(n-1-\frac{n}{2}+1\right) + 4^2(n-1-4) + (n-3)(n-2) \\ &= \frac{n^3}{4} + \frac{n^2}{4} + \frac{23n}{2} - 74 \leq Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right) \quad (n \geq 22). \end{aligned}$$

If the degree sequence of U_n is $\frac{n}{2}-1, \frac{n}{2}-1, 5, \overbrace{1, 1 \ldots 1}^{n-3}$, then we have

$$\begin{aligned} Lz(U_n) &= 2\left(\frac{n}{2}-1\right)^2\left(n-1-\frac{n}{2}+1\right)+5^2(n-1-5)+(n-3)(n-2) \\ &= \frac{n^3}{4}+21n-144 < Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right) \quad (n \geq 25). \end{aligned}$$

If the degree sequence of U_n is $\frac{n}{2}-1, \frac{n}{2}-1, 3, 3, \overbrace{1, 1 \ldots 1}^{n-4}$, then we have

$$\begin{aligned} Lz(U_n) &= 2\left(\frac{n}{2}-1\right)^2\left(n-1-\frac{n}{2}+1\right)+3^2(n-4)2+(n-4)(n-2) \\ &= \frac{n^3}{4}+13n-64 < Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right) \quad (n \geq 13). \end{aligned}$$

If the degree sequence of U_n is $\frac{n}{2}+1, \frac{n}{2}-1, 3, \overbrace{1, 1 \ldots 1}^{n-3}$, then we have

$$\begin{aligned} Lz(U_n) &= \left(\frac{n}{2}-1\right)^2\left(n-\frac{n}{2}\right)+\left(\frac{n}{2}+1\right)^2\left(n-\frac{n}{2}-2\right)+3^2(n-4)+(n-3)(n-2) \\ &= \frac{n^3}{4}+\frac{n^2}{2}+3n-32 < Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right). \end{aligned}$$

Case 3. Suppose that $\Delta > \frac{n}{2}-1$ and there is exactly one vertex v_1 with degree greater than $\frac{n}{2}-1$. Let $d(v_1)=\Delta=x_1>\frac{n}{2}-1$, $d(v_i)=x_i(2 \leq i \leq k)$ and $\lambda(x_2) \geq \ldots \geq \lambda(x_k)$, then there exists $x_1'(x_1' < \frac{n}{2}-1)$ such that $\lambda(x_1)=\lambda(x_1')$ by the symmetry of function $\lambda(x)$ (the proof is similar to Case 1). We have

$$\begin{aligned} Lz(U_n) &= \lambda(x_1)(x_1-1)+\lambda(x_2)(x_2-1)+\ldots+\lambda(x_k)(x_k-1) \\ &\leq \lambda\left(\frac{n}{2}-2\right)\left(\frac{n}{2}-3\right)+\lambda\left(\frac{n}{2}-2\right)\left(\frac{n}{2}-3\right)+6\lambda(7) < Lz\left(U_{\frac{n}{2},\frac{n}{2},3}\right). \end{aligned}$$

□

Lemma 3.5. *Let n be an even integer and U_n be a unicyclic graph with order n, where $n \geq 22$. If there is exactly one vertex v with $d(v)=2$ in U_n then $Lz(U_n) \leq \frac{n^3}{4}+\frac{3n^2}{4}-\frac{5n}{2}-8$ with equality if and only if $U_n \cong U_{\frac{n}{2}+1,\frac{n}{2},2}$.*

Proof. By Equation (2) we have

$$\begin{aligned} Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) &= \lambda\left(\frac{n}{2}\right)\left(\frac{n}{2}-1\right)+\lambda\left(\frac{n}{2}+1\right)\left(\frac{n}{2}+1-1\right)+\varphi(2) \\ &= \left(\frac{n^2}{4}+n-4\right)\left(\frac{n}{2}-1\right)+\left(\frac{n^2}{4}+n-7\right)\frac{n}{2}+\varphi(2) \\ &= \frac{n^3}{4}+\frac{3n^2}{4}-\frac{5n}{2}-8. \end{aligned}$$

Case 1. $\Delta \leq \frac{n}{2}-3$. Let $u_i \in R$, $d(u_i)=x_i \geq 3$ and $\lambda(x_1) \geq \ldots \geq \lambda(x_k)$. Then, we have

$$\begin{aligned} Lz(U_n) &= \lambda(x_1)(x_1-1)+\lambda(x_2)(x_2-1)+\ldots+\lambda(x_k)(x_k-1)+\varphi(2) \\ &\leq \lambda\left(\frac{n}{2}-3\right)(x_1-1)+\ldots+\lambda\left(\frac{n}{2}-3\right)(x_k-1)+\varphi(2) \quad \left(\text{as } \sum_{i=1}^{k}(x_i-1)=n-1\right) \\ &= \lambda\left(\frac{n}{2}-3\right)(n-1)+\varphi(2) \\ &= \left(\frac{n^2}{4}+n-7\right)(n-1)+4(n-3) \\ &= \frac{n^3}{4}+\frac{3n^2}{4}-4n-5 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}). \end{aligned}$$

Case 2. Suppose $\Delta \geq \frac{n}{2} - 2$.

Claim 2. There are at most two vertices of degree greater than or equal to $\frac{n}{2} - 2$.

Proof of Claim 2. Suppose that there exist $v_1 \dots v_l \in R$ $(l \geq 3)$ with $d(v_i) = x_i \geq \frac{n}{2} - 2$. Then, we have

$$\sum_{i=1}^{l}(x_i - 1) \geq 3\left(\frac{n}{2} - 2 - 1\right) = \frac{3n}{2} - 9 > n - 1,$$

which contradicts Equation (3). So, there are at most two vertices of degree greater than or equal to $\frac{n}{2} - 2$ in U_n.

Subcase 2.1. Assume that there are exactly two vertices of degree greater than or equal to $\frac{n}{2} - 2$, then by Equation (2), there are six possible cases.

Subcase 2.1.1. Suppose that U_n contains two vertices of degree $\frac{n}{2} - 1$. Then, the degree sequence of U_n is

$$\frac{n}{2} - 1, \frac{n}{2} - 1, 4, 2, \overbrace{1 \dots 1}^{n-4}$$

and thus

$$\begin{aligned} Lz(U_n) &= 2\left(\frac{n}{2} - 1\right)^2\left(n - 1 - \frac{n}{2} + 1\right) + 4^2(n-5) + 2^2(n-3) + (n-4)(n-2) \\ &= \frac{n^3}{4} + 15n - 84 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 21). \end{aligned}$$

Subcase 2.1.2. Suppose that U_n contains a vertex of degree $\frac{n}{2} - 1$ and a vertex of degree $\frac{n}{2}$. The degree sequence of U_n is

$$\frac{n}{2}, \frac{n}{2} - 1, 3, 2, \overbrace{1 \dots 1}^{n-4}$$

and thus

$$\begin{aligned} Lz(U_n) &= \left(\frac{n}{2} - 1\right)^2\left(n - \frac{n}{2}\right) + \left(\frac{n}{2}\right)^2\left(n - 1 - \frac{n}{2}\right) + 3^2(n-4) + 2^2(n-3) + (n-4)(n-2) \\ &= \frac{n^3}{4} + \frac{n^2}{4} + \frac{15n}{2} - 40 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 16). \end{aligned}$$

Subcase 2.1.3. Suppose that U_n has a vertex of degree $\frac{n}{2} - 1$ and a vertex of degree $\frac{n}{2} - 2$. The degree sequence of U_n is

$$\frac{n}{2} - 1, \frac{n}{2} - 2, 3, 3, 2\,\overbrace{1 \dots 1}^{n-5} \quad \text{or} \quad \frac{n}{2} - 1, \frac{n}{2} - 2, 5, 2, \overbrace{1 \dots 1}^{n-4}.$$

If the degree sequence of U_n is $\frac{n}{2} - 1, \frac{n}{2} - 2, 3, 3, 2, \overbrace{1 \dots 1}^{n-5}$, then we get

$$\begin{aligned} Lz(U_n) &= \left(\frac{n}{2} - 1\right)^2\frac{n}{2} + \left(\frac{n}{2} - 2\right)^2\left(\frac{n}{2} + 1\right) + 2 \times 3^2(n-4) + 2^2(n-3) + (n-5)(n-2) \\ &= \frac{n^3}{4} - \frac{n^2}{4} + \frac{31n}{2} - 70 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 16). \end{aligned}$$

If the degree sequence of U_n is $\frac{n}{2} - 1, \frac{n}{2} - 2, 5, 2, \overbrace{1 \dots 1}^{n-4}$, then we get

$$Lz(U_n) = \frac{n^3}{4} - \frac{n^2}{4} + \frac{47n}{2} - 150 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 21).$$

Subcase 2.1.4. Suppose that U_n has a vertex of degree $\frac{n}{2}$ and a vertex of degree $\frac{n}{2} - 2$. Then, the degree sequence of U_n is

$$\frac{n}{2}, \frac{n}{2} - 2, 4, 2, \overbrace{1 \dots 1}^{n-4}$$

and thus

$$Lz(U_n) = \frac{n^3}{4} + 14n - 80 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 19).$$

Subcase 2.1.5. Suppose that U_n contains two vertices of degree $\frac{n}{2}-2$, then the degree sequence of U_n is

$$\frac{n}{2}-2, \frac{n}{2}-2, 6, 2, \overbrace{1\ldots1}^{n-4} \quad \text{or} \quad \frac{n}{2}-2, \frac{n}{2}-2, 4, 3, 2, \overbrace{1\ldots1}^{n-5}.$$

If the degree sequence of U_n is $\frac{n}{2}-2, \frac{n}{2}-2, 6, 2, \overbrace{1\ldots1}^{n-4}$, then we get

$$Lz(U_n) = \frac{n^3}{4} - \frac{n^2}{2} + 34n - 248 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 22).$$

If the degree sequence of U_n is $\frac{n}{2}-2, \frac{n}{2}-2, 4, 3, 2, \overbrace{1\ldots1}^{n-5}$, then we get

$$Lz(U_n) = \frac{n^3}{4} - \frac{n^2}{2} + 18n - 98 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 11).$$

Subcase 2.1.6. Suppose that U_n has a vertex of degree $\frac{n}{2}+1$ and a vertex of degree $\frac{n}{2}-2$. The degree sequence of U_n is

$$\frac{n}{2}+1, \frac{n}{2}-2, 3, 2, \overbrace{1\ldots1}^{n-4}$$

and thus

$$Lz(U_n) = \frac{n^3}{4} + \frac{n^2}{4} + \frac{11n}{2} - 38 \leq Lz(U_{\frac{n}{2}+1,\frac{n}{2},1}) \quad (n \geq 15).$$

Subcase 2.2. Suppose that there is only one vertex v_1 with $d(v_1) = \Delta = x_1 \geq \frac{n}{2}-2$. Let $d(v_i) = x_i (2 \leq i \leq l)$ and $\lambda(x_2) \geq \ldots \lambda(x_l)$. Then,

$$\begin{aligned} Lz(U_n) &= \lambda(x_1)(x_1-1) + \ldots + \lambda(x_l)(x_l-1) + \varphi(2) \\ &\leq 2\lambda\left(\frac{n}{2}-1\right)\left(\frac{n}{2}-2\right) + \lambda(4)(4-1) + \varphi(2) < Lz(U_{\frac{n}{2}+1,\frac{n}{2},2}) \quad (n \geq 21). \end{aligned}$$

□

Lemma 3.6. *Let n be an odd integer and U_n be a unicyclic graph with n vertices, where $n > 26$. If there is no vertex v with $d(v) = 2$ in U_n, then $Lz(U_n) \leq \frac{n^3}{4} + \frac{n^2}{2} + \frac{15n}{4} - \frac{61}{2}$ with equality if and only if $U_n \cong U_{\frac{n-1}{2},\frac{n+1}{2},3}$.*

Proof. By Equation (2), we have

$$\begin{aligned} Lz(U_{\frac{n-1}{2},\frac{n+1}{2},3}) &= \lambda\left(\frac{n-1}{2}\right)\left(\frac{n-1}{2}-1\right) + \lambda\left(\frac{n+1}{2}\right)\left(\frac{n+1}{2}-1\right) + \lambda(3)(3-1) \\ &= \frac{n^3}{4} + \frac{n^2}{2} + \frac{15n}{4} - \frac{61}{2}. \end{aligned}$$

Case 1. Suppose $\Delta \leq \frac{n-3}{2}$ and there is at most one vertex of degree $\frac{n-3}{2}$. Let $u_i \in R$, $d_{u_i} = x_i \geq 3$ and $\lambda(x_1) \geq \ldots \geq \lambda(x_k)$, then we have

$$\begin{aligned} Lz(U_n) &= \lambda(x_1)(x_1-1) + \lambda(x_2)(x_2-1) + \ldots + \lambda(x_k)(x_k-1) \quad \left(\text{as } \sum_{i=1}^{k}(x_i-1) = n\right) \\ &\leq \lambda(x_1)\left(\frac{n-1}{2}-1\right) + \lambda(x_2)\left(\frac{n+1}{2}-1\right) + 2\lambda(x_k) \\ &< \lambda\left(\frac{n-1}{2}\right)\left(\frac{n-1}{2}-1\right) + \lambda\left(\frac{n+1}{2}\right)\left(\frac{n+1}{2}-1\right) + 2\lambda(3) \\ &= Lz(U_{\frac{n-1}{2},\frac{n+1}{2},3}). \end{aligned}$$

Case 2. Suppose $\Delta \geq \frac{n-3}{2}$ and there are at least two vertices of degree greater than or equal to $\frac{n-3}{2}$.

Claim 3: There are at most two vertices of degree greater than or equal to $\frac{n-3}{2}$.

Proof of Claim 3. Suppose that there exist $v_1, \cdots, v_l \in R$ $(l \geq 3)$ with $d(v_i) = x_i \geq \frac{n-3}{2}$. Then, we have

$$\sum_{i=1}^{l}(x_i - 1) \geq 3\left(\frac{n-3}{2} - 1\right) = \frac{3n}{2} - \frac{11}{2} > n,$$

which is a contradiction to Equation (3). So, there are at most two vertices of degree greater than or equal to $\frac{n-3}{2}$ in U_n.

By Equation (3) and Claim 3, we only consider the next five cases.

Subcase 2.1. Assume that U_n contains a vertex of degree $\frac{n-3}{2}$ and a vertex of degree $\frac{n-1}{2}$, then the degree sequences of U_n has two possible cases:

(i) Suppose that the degree sequence of U_n is $\frac{n-1}{2}, \frac{n-3}{2}, 5, \overbrace{1, 1 \ldots 1}^{n-3}$, then we get

$$Lz(U_n) = \frac{n^3}{4} + \frac{83n}{4} - 143 \leq Lz(U_{\frac{n+1}{2}, \frac{n-1}{2}, 3}) \quad (n \geq 25).$$

(ii) Suppose that the degree sequence of U_n is $\frac{n-3}{2}, \frac{n-1}{2}, 3, 3, \overbrace{1, 1 \ldots 1}^{n-4}$, then we get

$$Lz(U_n) = \frac{n^3}{4} + \frac{51n}{4} - 63 \leq Lz(U_{\frac{n+1}{2}, \frac{n-1}{2}, 3}).$$

Subcase 2.2. Suppose that U_n has a vertex of degree $\frac{n-3}{2}$ and a vertex of degree $\frac{n+1}{2}$, then the degree sequence of U_n is

$$\frac{n+1}{2}, \frac{n-3}{2}, 4, \overbrace{1, 1 \ldots 1}^{n-3}$$

and thus

$$Lz(U_n) = \frac{n^3}{4} + \frac{n^2}{4} + \frac{43n}{4} - \frac{293}{4} \leq Lz(U_{\frac{n-1}{2}, \frac{n+1}{2}, 3}) \quad (n \geq 19).$$

Subcase 2.3. Suppose that U_n has a vertex of degree $\frac{n-3}{2}$ and a vertex of degree $\frac{n+3}{2}$, then the degree sequence of U_n is

$$\frac{n+3}{2}, \frac{n-3}{2}, 3, \overbrace{1, 1 \ldots 1}^{n-3}$$

and thus

$$Lz(U_n) = \frac{n^3}{4} + \frac{n^2}{2} + \frac{7n}{4} - \frac{69}{2} < Lz(U_{\frac{n-1}{2}, \frac{n+1}{2}, 3}).$$

Subcase 2.4. Suppose that U_n has two vertices of degree $\frac{n-3}{2}$, then the degree sequences of U_n have two possible cases:

(i) Suppose that the degree sequence of U_n is $\frac{n-3}{2}, \frac{n-3}{2}, 6, \overbrace{1, 1 \ldots 1}^{n-3}$, then we obtain

$$Lz(U_n) = \frac{n^3}{4} - \frac{n^2}{4} + \frac{127n}{4} - \frac{975}{4} < Lz(U_{\frac{n-1}{2}, \frac{n+1}{2}, 3}) \quad (n > 26).$$

(ii) Suppose that the degree sequence of U_n is $\frac{n-3}{2}, \frac{n-3}{2}, 4, 3, \overbrace{1, 1 \ldots 1}^{n-4}$, then we obtain

$$Lz(U_n) = \frac{n^3}{4} - \frac{n^2}{4} + \frac{79n}{4} - \frac{423}{4} < Lz(U_{\frac{n-1}{2}, \frac{n+1}{2}, 3}) \quad (n \geq 15).$$

Subcase 2.5. Suppose that U_n contains two vertices of degree $\frac{n-1}{2}$, then the degree sequence of U_n is

$$\frac{n-1}{2}, \frac{n-1}{2}, 4, \overbrace{1, 1 \ldots 1}^{n-3}$$

and thus

$$Lz(U_n) = \frac{n^3}{4} + \frac{n^2}{4} + \frac{47n}{4} - \frac{297}{4} \leq Lz(U_{\frac{n-1}{2}, \frac{n+1}{2}, 3}) \quad (n \geq 25).$$

Case 3. Suppose $\Delta > \frac{n-3}{2}$ and assume that there is only one vertex v_1 with degree greater than $\frac{n-3}{2}$. By the arguments similar to the ones provided in the proof of Case 3 of Lemma 3.2, we have $Lz(U_n) \leq Lz(U_{\frac{n-1}{2}, \frac{n+1}{2}, 3})$.

□

Lemma 3.7. *Let n be an odd integer and U_n be a unicyclic graph with order n, where $n \geq 19$. If there is exactly one vertex v with $d(v) = 2$ in U_n, then $Lz(U_n) \leq \frac{n^3}{4} + \frac{3n^2}{4} + \frac{35n}{4} - \frac{191}{4}$ with equality if and only if $U_n \cong U_{\frac{n+1}{2},\frac{n+1}{2},2}$.*

Proof. By Equation (2), we have

$$Lz(U_{\frac{n-1}{2},\frac{n+3}{2},2}) = \frac{n^3}{4} + \frac{3n^2}{4} - \frac{9n}{4} - \frac{27}{4}.$$

Case 1. Suppose $\Delta < \frac{n-3}{2}$. Let $u_i \in R$, $d(u_i) = x_i \geq 3$ and $\lambda(x_1) \geq \lambda(x_2) \ldots \lambda(x_k)$. Then, we get

$$\begin{aligned} Lz(U_{\frac{n+1}{2},\frac{n+1}{2},2}) &= \lambda(x_1)(x_1-1) + \ldots + \lambda(x_k)(x_k-1) + \varphi(2) \quad \left(\text{as } \sum_{i=1}^{k}(x_i-1) = n-1\right) \\ &\leq \lambda(x_1)\left(\frac{n+1}{2}-1\right) + \lambda(x_2)\left(\frac{n+1}{2}-1\right) + \varphi(2) \\ &< \lambda\left(\frac{n-5}{2}\right)\left(\frac{n+1}{2}-1\right) + \lambda\left(\frac{n-5}{2}\right)\left(\frac{n+1}{2}-1\right) + \varphi(2) \\ &= Lz(U_{\frac{n+1}{2},\frac{n+1}{2},2}). \end{aligned}$$

Case 2. Suppose $\Delta \geq \frac{n-3}{2}$.

Claim 4. There are at most two vertices of degree greater than or equal to $\frac{n-3}{2}$.

Proof of Claim 4. Suppose that there exist $v_1, \cdots, v_l \in R$ $(l \geq 3)$ with $d(v_i) = x_i \geq \frac{n-3}{2}$, then we have

$$\sum_{i=1}^{l}(x_i-1) \geq 3\left(\frac{n-3}{2}-1\right) = \frac{3n}{2} - \frac{11}{2} > n-1,$$

which contradicts (2). So, there are at most two vertices of degree greater than or equal to $\frac{n-3}{2}$ in U_n.

Subcase 2.1. Suppose that there are two vertices of degree great than or equal to $\frac{n-3}{2}$. Then, we attain the following situations by (2).

Subcase 2.1.1. Suppose that U_n has two vertices of degree $\frac{n-3}{2}$, then the degree sequence of U_n is $\frac{n-3}{2}, \frac{n-3}{2}, 5, 2, \overbrace{1, 1 \ldots 1}^{n-4}$ and thus

$$Lz(U_n) = \frac{n^3}{4} - \frac{n^2}{4} + \frac{95n}{4} - \frac{607}{4} < Lz(U_{\frac{n+1}{2},\frac{n+1}{2},2}) \quad (n \geq 18).$$

Subcase 2.1.2. Suppose that U_n has a vertex of degree $\frac{n-3}{2}$ and a vertex of degree $\frac{n-1}{2}$, then the degree sequence of U_n is

$$\frac{n-3}{2}, \frac{n-1}{2}, 4, 2, \overbrace{1, 1 \ldots 1}^{n-4}$$

and thus

$$Lz(U_n) = \frac{n^3}{4} + \frac{59n}{4} - 83 < Lz(U_{\frac{n+1}{2},\frac{n+1}{2},2}) \quad (n \geq 17).$$

Subcase 2.1.3. Suppose that U_n has a vertex of degree $\frac{n-3}{2}$ and a vertex of degree $\frac{n+1}{2}$, then the degree sequence of U_n is

$$\frac{n+1}{2}, \frac{n-3}{2}, 3, 2, \overbrace{1, 1 \ldots 1}^{n-4}$$

and hence

$$Lz(U_n) = \frac{n^3}{4} + \frac{n^2}{4} + \frac{27n}{4} - \frac{157}{4} < Lz(U_{\frac{n+1}{2},\frac{n+1}{2},2}) \quad (n \geq 13).$$

Subcase 2.1.4. Suppose that U_n has two vertices of degree $\frac{n-1}{2}$, then the degree sequence of U_n is $\frac{n-1}{2}, \frac{n-1}{2}, 3, 2, \overbrace{1, 1 \ldots 1}^{n-4}$ and hence

$$Lz(U_n) = \frac{n^3}{4} + \frac{n^2}{4} + \frac{31n}{4} - \frac{161}{4} < Lz(U_{\frac{n+1}{2},\frac{n+1}{2},2}) \quad (n \geq 16).$$

Subcase 2.1.5. Suppose that U_n has two vertices of degree $\frac{n+1}{2}$, then the degree sequence of U_n is $\frac{n-1}{2}, \frac{n+3}{2}, 2, \overbrace{1, 1 \ldots 1}^{n-3}$ and thus

$$Lz(U_n) = \frac{n^3}{4} + \frac{3n^2}{4} - \frac{13n}{4} - \frac{47}{4} < Lz(U_{\frac{n+1}{2}, \frac{n+1}{2}, 2}).$$

Subcase 2.2. Suppose that there is only one vertex of degree greater than or equal to $\frac{n-3}{2}$. By the reasoning similar to one provided in the proof of Case 3 of Lemma 3.2, we have $Lz(U_n) \leq Lz(U_{\frac{n+1}{2}, \frac{n+1}{2}, 2})$. $\square$

By Lemmas 3.4–3.7, we have next result.

Theorem 3.1. *Let U_n be a unicyclic graph of order n, where $n \geq 26$.*

(i). *If n is even, then $Lz(U_n) \leq \frac{n^3}{4} + \frac{3n^2}{4} - \frac{5n}{2} - 8$ with equality if and only if $U_n \cong U_{\frac{n}{2}+1, \frac{n}{2}, 2}$.*

(ii). *If n is odd, then $Lz(U_n) \leq \frac{n^3}{4} + \frac{3n^2}{4} + \frac{35n}{4} - \frac{19}{4}$ with equality if and only if $U_n \cong U_{\frac{n+1}{2}, \frac{n+1}{2}, 2}$.*

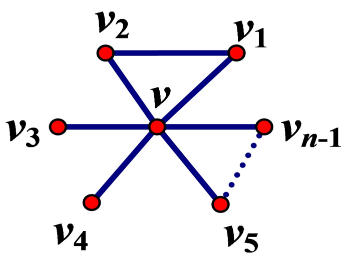

Figure 2: The graph $S_n + e$.

Theorem 3.2. *Let U_n be a unicyclic graph with n vertices, then $Lz(U_n) \geq n^2 + 3n - 18$ with equality if and only if $U_n \cong S_n + e$ (see Figure 2).*

Proof. Let $V(U_n) = R \cup L$, where $R = \{v \in V(U_n) \mid d(v) > 1\}$ and $L = \{v \in V(U_n) \mid d(v) = 1\}$. Take $|R| = r$ and $|L| = l$. Since

$$\sum_{u \in R} d(u) + l = 2n,$$

we attain

$$\sum_{u \in R} (d(u) - 2) = l,$$

$$\sum_{u \in R} (d(u) - 1) = n. \tag{4}$$

Let $c(x) = x^2(n-1-x)$ and

$$f(x) = \frac{c(x) + (x-2)c(1)}{x-1} = -x^2 + (n-2)x + 2(n-2).$$

We have $f(x)_{min} = f(n-1) = n-3$. In the remaining proof, we take $d_u = d(u)$ for simplicity. By the definition of the Lanzhou index and Equation (4), we have

$$\begin{aligned}
Lz(U_n) &= \sum_{u \in R} c(d_u) + l\, c(1) \\
&= \sum_{u \in R} c(d_u) + \sum_{u \in R} (d_u - 2)c(1) \\
&= \sum_{u \in R} \Big(c(d_u) + (d_u - 2)c(1) \Big) \\
&= \sum_{u \in R} \frac{c(d_u) + (d_u - 2)c(1)}{d_u - 1}(d_u - 1) \\
&\geq f(d_u)_{min} \sum_{u \in R} (d_u - 1) \\
&= (n-3)n.
\end{aligned}$$

If there is no vertex of degree $n-1$ in U_n, then

$$Lz(U_n)_{min} \geq f(n-2)\sum_{u\in R}(d_u-1) = 2n^2-4n > n^2+3n-18 \ \ (n \geq 3).$$

If there is a vertex of degree $n-1$ in U_n, then $U_n \cong S_n + e$ and

$$Lz(S_n+e) = (n-3)(n-2) + 2^2(n-3) + 2^2(n-3) = n^2+3n-18.$$

□

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