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The Lanzhou Index of Unicyclic Graphs with Fixed Maximum Degree

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Abstract

For a graph G with vertex set $V(G)$ and edge set $E(G)$, the Lanzhou index of G is defined as

$$Lz(G) = \sum_{v \in V(G)} d_G(v)^2 d_{\overline{G}}(v),$$

where $d_G(v)$ is the degree of vertex v in G, $\overline{G}$ is the complement of G. Vukičević, Li, Sedlar and Došlić [MATCH Commun. Math. Comput. Chem. 86 (2021) 3–10] proved that for any tree T of order $n \geq 11$ with maximum degree Δ, $Lz(T) \geq (n - \Delta - 1)(4n + \Delta^2 - 12) + \Delta(n - 2)$. In this paper, we generalize the foregoing bound and we show that for any unicyclic graph U of order $n \geq 11$ with maximum degree Δ, $Lz(U) \geq 4(n-3)(n-\Delta+1)+\Delta^2(n-1-\Delta)+(n-2)(\Delta-2)$, and we also characterize the corresponding extremal unicyclic graphs.

1 Introduction

In this paper, we consider only simple, finite and undirected graphs. Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v \in V(G)$ is equal to the number of its

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neighbors and we denote it by $d_G(v)$. A vertex of degree 1 is called a *leaf*. We denote by $\Delta(G)$ and $\Delta'(G)$ the maximum and second maximum degree of the vertices of G. For any $u \in V(G)$, the neighborhood of u, written as $N_G(u)$, is the set of vertices adjacent to u. The *complement graph* $\overline{G}$ of G has the same vertex set $V(G)$, and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G. Let $G = (V, E)$ be a connect graph. If $W \subseteq V(G)$, we denote by $G - W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. If $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E'. If $W = \{v\}$ and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v$ and $G - xy$ for short. Let $G + uv$ denote the graph obtained from G by adding the edge $uv \notin E(G)$. We denote by $U_{n,\Delta}$ the set of unicyclic graphs of order n and maximum degree Δ. The complete graph, the cycle, the path and the star on n vertices are denoted by K_n, C_n, P_n and S_n. A spider is a tree with at most one vertex of degree more than 2, called the *center* of the spider (if no vertex is of degree more than two, then any vertex can be the *center*). A leg of a spider is a path from the center to a vertex of degree 1. The star S_n is a spider of $n - 1$ legs, each of length 1, the path P_n is a spider of 1 or 2 legs. For other undefined notations and terminology from graph theory, the readers are referred to [1].

The first Zagreb index $M_1(G)$ of a graph G is defined as

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

while the Forgotten index of G is defined as

$$F(G) = \sum_{v \in V(G)} d_G(v)^3.$$

They were defined in the same paper [7]. The mathematical and chemical properties of the first Zagreb index have been studied in [2–4,8]. Forgotten index was reintroduced by Furtula and Gutman in [5].

In 2018, researchers Vukičević, Li, Sedlar and Došlić, proposed a new topological index. When they came to Lanzhou for communication, they showed that it behaves better than the existing ones in predicting a chemically relevant property. It is put forward according to $Furtula - Gutman$ linear combination $M_1(G) + \lambda F(G)$, where λ was a free parameter ranging from -20 to 20. A sharp peak was obtained at $\lambda = -0.140$ [6]. Later, Vukičević et al, found that the absolute value of λ was very close to $\frac{1}{7}$, and the value of the denominator is the largest possible degree of a vertex in octanes with 8 vertices, but nonanes are molecular graphs with 9 vertices. Therefore, Vukičević et al. defined a new index for a molecular graph G named the Lanzhou index [6], which is denoted by $Lz(G)$. They first interpret the free parameter λ as $\frac{-1}{n-1}$ in the Furtula-Gutman linear combination, then multiply $n-1$ to get rid of fractions. That is,

$$\begin{aligned} Lz(G) &= (n-1)(M_1(G) - F(G)) \\ &= \sum_{v \in V(G)} d_G(v)^2[(n-1) - d_G(v)] \\ &= \sum_{v \in V(G)} d_G(v)^2 d_{\overline{G}}(v). \end{aligned}$$

As is well known, finding extremal graphs and values of the topological indices over some classes of graphs attracts the attention of many researchers. In [6], extremal graphs with n vertices are illustrated. More precisely, complete and empty graphs are of minimum Lanzhou index 0, and $\frac{2}{3}(n-1)$-regular graphs with $n \equiv 1 (\mathrm{mod}\ 3)$ are of maximum Lanzhou index $\frac{4}{27}n(n-1)^3$. For trees with n vertices, star and balanced double star are the minimal and maximal graphs respectively.

Recently, many scholars have paid great attention to Lanzhou index.

Theorem 1. [6] For any tree T of order $n \geq 15$, then

$$Lz(T) \geq (n-1)(n-2),$$

with equality if and only if $T = S_n$.

Theorem 2. [6] For any tree T of order n with maximum degree at most 4, then

$$Lz(T) \geq 4n^2 - 18n + 20,$$

with equality if and only if $T = P_n$.

Theorem 3. [11] For any tree T of order $n \geq 11$ with maximum degree Δ. Then

$$Lz(T) \geq (n-1-\Delta)(4n+\Delta^2-12)+\Delta(n-2),$$

with equality if and only if T is a spider with the center of degree Δ.

Theorem 4. [9] For any tree $T \in T(n, \Delta, \Delta')$ with $n \geq 11$. Then

$$Lz(T) \geq (n-1)(\Delta^2+\Delta'^2)-(\Delta^3+\Delta'^3)-(3n-10)(\Delta+\Delta')+(4n^2-14n+4)$$

with equality if and only if T is a double spider with the degrees of center Δ and Δ'.

In 2019 [10], Liu et al. proved the extreme value and the extremal graph of the Lanzhou index of the unicyclic graph.

Therefore, in this paper we establish a best possible lower bound for the Lanzhou index of unicyclic graphs in terms of their order and maximum degree and characterize all extreme trees, as a generalization of aforementioned result.

2 Unicyclic graphs

In this section, we present a sharp lower bound for the Lanzhou index of unicyclic graphs in terms of their order and maximum degree. We also characterize all unicyclic graphs whose Lanzhou index achieves the lower bound.

Transformation A. Let G is a unicyclic graph of order n with its unique cycle C_k. Let T_{u_0} be a pendent tree of G attaching to the vertex $u_0 \in V(C_k)$. For a vertex $v_0 \in T_{u_0}$ not on C_k with $d_G(v_0) \geq 2$. Let y be a vertex on the path between u_0 and v_0 such that y is adjacent to v_0, and $v_1, \cdots, v_t$ be other neighbors of v_0, $u_1u_2 \in E(C_k)$. Let $G' = G - \{yv_0, v_0v_t, u_1u_2\} + \{yv_t, u_1v_0, u_2v_0\}$. Therefore, v_0 is on the cycle of graph G', and $d_G(v_0) = d_{G'}(v_0)$. For example, see Figure 1.

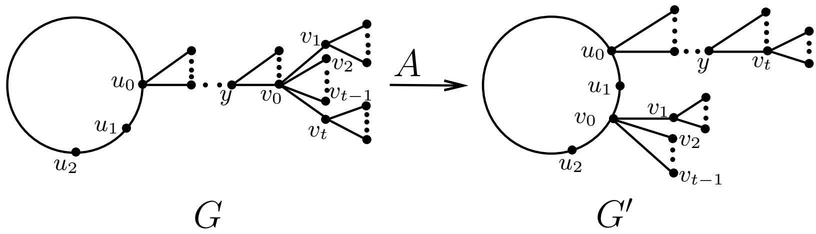

Figure 1. Transformation A from graph G to G'

Remark 5. *It is easily seen that any unicyclic graph G can be changed into a unicyclic graph G' with maximum degree on cycle C_k by repeating Transformation A. During this process, we can see that graphs G and G' have the same degree sequence, so $Lz(G) = Lz(G')$.*

Transformation B. Suppose that G is a connected graph of order $n \geq 11$ with maximum degree Δ. Let $u_0,\ h_0 \in V(G)$, $P' = u_0u_1u_2, \cdots, u_k$ and $P'' = h_0h_1h_2, \cdots, h_s$ are two pendent paths in G, respectively, where $k,\ s \geq 1$, and $u_k,\ h_s$ are are pendant vertices of G. Let $G' = G - h_0h_1 + u_kh_1$. Hence $V(G) = V(G') = n \geq 11$, and $d_G(u_k) = 1$ $d_{G'}(u_k) = 2$. Assume that $d_G(h_0) = t \geq 3$, $d_{G'}(h_0) = t - 1$, and for any $v \in V(G)\backslash\{u_k,\ h_0\}$, $d_G(v) = d_{G'}(v)$. The above referred graphs have been illustrated in Figure 2.

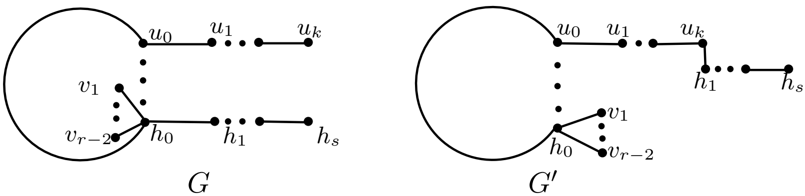

Figure 2. Transformation B from graph G to G'

Proposition 6. *Let G' be obtained from a connected graph G by Transformation B. Then G' is also a connected graph, and $Lz(G') < Lz(G)$.*

Proof. Applying transformation B, we know that the degrees of all vertices in graph G and graph G' except for vertices h_0 and u_k have not changed.

So, let $D = \{h_0,\ u_k\}$, then

$$Lz(G) - Lz(G') = \sum_{w \in D} [d_G(w)^2(n-1-d_G(w)^2)] - [d_{G'}(w)^2(n-1-d_{G'}(w)^2))].$$

(I) If $h_0 = u_0$, $k = s = 1$, and $h_1 = v_{r-2}$, then

$$\begin{aligned} Lz(G) - Lz(G') &= t^2(n-1-t) + 1^2(n-2) - (t-1)^2(n-t) - 2^2(n-3) \\ &= t^2(n-1-t) - (t-1)^2(n-t) + (n-2) - 4(n-3) \\ &= -3t^2 + 2tn - 4n + t + 10 \\ &= 2n(t-2) - 3t^2 + t + 10. \end{aligned}$$

Since $n \geq 2t$, Suppose $n = 2t + y$ (y is a non-negative integer). Then we have

$$\begin{aligned} Lz(G) - Lz(G') &= 2n(t-2) - 3t^2 + t + 10 \\ &= t^2 + (2y-7)t - 4y + 10 \qquad (1) \\ &= (t+2y-5)(t-2). \end{aligned}$$

Since $t \geq 3$, so $t + 2y \geq 7$ when $y \geq 2$ and hence from (1), we have $Lz(G) - Lz(G') > 0$ when $y \geq 2$. Again since $n \geq 11$ and $n = 2t + y$, so $t \geq 6$ and $t \geq 5$ according to $y = 0$ and $y = 1$. Thus in this case, we have $t + 2y \geq 6$ and hence we have $Lz(G) - Lz(G') > 0$ in the case when $y = 0, 1$.

(II) If $h_0 \neq u_0$ and $k = s = 1$, then

$$Lz(G) - Lz(G') = t^2(n-1-t) - (t-1)^2(n-t) + (n-2) - 4(n-3) \qquad (2)$$

By Eq. (2) and the fact that $n \geq 2t + 2$, and similar to the proof of type (I), we can obtain $Lz(G) - Lz(G') > 0$.

(III) If $h_0 \neq u_0$ and $k, s \geq 2$, then

$$Lz(G) - Lz(G') = t^2(n-1-t) - (t-1)^2(n-t) + (n-2) - 4(n-3). \qquad (3)$$

By Eq. (3) and the fact that $n \geq 2t + k + s$, and similar to the proof of type (I), we can obtain $Lz(G) - Lz(G') > 0$.

This completes the proof. ■

Let $U \in U_{n,\Delta}$, C is the unique cycle of graph U. If $U - E(C)$ is some independent vertices and a spider, which center is on cycle C and has $\Delta - 2$

legs, then denote the set of such graphs as $U^S_{n,\Delta}$. For any $G \in U^S_{n,\Delta}$, then it's easy to get the following results.

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

Theorem 7. *Let U be a unicyclic graph of $n \geq 11$ with maximum degree Δ,*

$$Lz(U) \geq 4(n-3)(n-\Delta+1) + \Delta^2(n-1-\Delta) + (n-2)(\Delta-2),$$

with equality holding if and only if $U \in U^S_{n,\Delta}$.

Proof. Let U be a unicyclic graph of $n \geq 11$ with maximum degree Δ. If $\Delta = 2$, then U is a cycle C_k of order n.

$$Lz(U) = 4n^2 - 12n = 4(n-3)(n-\Delta+1) + \Delta^2(n-1-\Delta) + (n-2)(\Delta-2).$$

Now let $\Delta \geq 3$. According to Remark 5, any unicyclic graph U can be changed into a unicyclic graph U' with maximum degree on cycle C_k. Repeating applying transformation B, any unicyclic graph U can become a unicyclic graph belonging to $U^S_{n,\Delta}$. Hence

$$Lz(U) \geq 4(n-3)(n-\Delta+1) + \Delta^2(n-1-\Delta) + (n-2)(\Delta-2).$$

This completes the proof of Theorem 7. ■

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