Research Article

On the Maximal-Adjacency-Spectrum Unicyclic Graphs with Given Maximum Degree

Haizhou Song\(^1\) and Lulu Tian\(^2\)

\(^1\)College of Mathematical Sciences, Huaqiao University, Quanzhou, Fujian 362021, China
\(^2\)Shanghai Aerospace Control Technology Institute, Shanghai 201109, China

Correspondence should be addressed to Haizhou Song; hzsong@hqu.edu.cn

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In this paper, we study the properties and structure of the maximal-adjacency-spectrum unicyclic graphs with given maximum degree. We obtain some necessary conditions on the maximal-adjacency-spectrum unicyclic graphs in the set of unicyclic graphs with \(n\) vertices and maximum degree \(\Delta\) and describe the structure of the maximal-adjacency-spectrum unicyclic graphs in the set. Besides, we also give a new upper bound on the adjacency spectral radius of unicyclic graphs, and this new upper bound is the best upper bound expressed by vertices \(n\) and maximum degree \(\Delta\) from now on.

1. Introduction

The spectral theory of graphs was established in the 1940s and 1950s. It is a branch of mathematics that is widely applied, and it is a powerful tool for solving problems in discrete mathematics. Many of the early results were related to the relationship between the spectrum and the structural properties of a graph [1–4]. The spectral theory of graphs has been widely used in quantum theory, chemistry, physics, computer science, the theory of communication networks, and information science. Along with the continuous research of the spectral theory of graphs, applications of the spectral theory of graphs have also been found in the fields of electrical networks and vibration theory [5, 6].

Not only has the spectral theory of graphs pushed forward and enriched research into combinatorics and graph theory but also it has been widely used in quantum theory, chemistry, physics, computer science, the theory of communication networks, and information science. The wide range of application of the spectral theory of graphs has led to the spectral theory of graphs becoming a very active field of research over the last thirty to forty years, and large numbers of results are continuously emerging.

There are many results on the adjacency spectral radius for different classes of graphs. Guo et al. [7] have studied the largest and the second largest spectral radius of trees with \(n\) vertices and diameter \(d\). Guo and Shao [8] have studied the first \(\lfloor d/2 \rfloor + 1\) spectral radii of graphs with \(n\) vertices and diameter \(d\). Petrovic et al. [9, 10] have studied the spectral radius of unicyclic and bicyclic graphs with \(n\) vertices and \(k\) pendant vertices. Guo et al. [11, 12] have studied the spectral radius of unicyclic and bicyclic graphs with \(n\) vertices and diameter \(d\).

Let \(T = (V, E)\) be a connected graph with edge set \(E\) and vertex set \(V\). In this paper, we denote by \((u, v)\) a edge of \(E\), where \(u \in V, v \in V\). Denote the maximum degree of vertex \(T\) by \(\Delta(T)\). For convenience, we shall sometimes denote \(\Delta(T)\) simply by \(\Delta\). Denote the degree of vertex \(v\) by \(d(v)\). Denote by \(N_T(v)\) the set which consists of the vertices adjacent to vertex \(v\) in \(T\). Denote by \(d(u, v)\) the shortest distance between vertex \(u\) and vertex \(v\). Denote by \(\rho(T)\) the adjacency spectral radius of \(T\). If \(T = (V, E)\) is a connected graph with \(n\) vertices, where \(V\) is the vertex set of \(T\), \(E\) is the edge set of \(T\), and \(|E| = n\), then \(T\) is called a unicyclic graph. We denote the set which consists of the unicyclic graphs with \(n\) vertices and maximum degree \(\Delta\) by \(T^n_\Delta\).
In this paper, we study further the properties and structure of the maximal-adjacency-spectrum unicyclic graphs in the set of unicyclic graphs with \( n \) vertices and the maximum degree \( \Delta \), where \( \Delta \geq 3 \). Besides, we study the new upper bound on the adjacency spectral radius of unicyclic graphs.

Suppose that \( T^* \in T_n^\Delta \), then we obtain some necessary conditions that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph with \( n \) vertices and the maximum degree \( \Delta \).

**Theorem 1.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \) if \( x = (x_1, x_2, \ldots, x_n)^T \) is the Perron vector of \( T^* \), then the degree of the vertices that corresponds to all largest components in the component of \( x \) is \( \Delta \).

**Theorem 2.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \) and the only circle in \( T^* \) is \( C \), \( x = (x_1, x_2, \ldots, x_n)^T \) is the Perron vector of \( T^* \); if the component of \( x \), which corresponds to the vertex \( u \) in \( x \) satisfies that \( x_{u^*} = \max_{i \in \text{circ}(u)} x_i \), then \( u^* \in V(C) \).

**Theorem 3.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \), if the only circle in \( T^* \) is \( C \), and there exists a nonfull internal vertex in the set of \( V(T^*) \setminus V(C) \), then the number of all the nonfull internal vertices of \( T^* \) is one.

**Theorem 4.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \), let \( C \) be the only circle in \( T^* \) and \( |V(C)| = 3 \), if there is no nonfull internal vertex in the set of \( V(T^*) \setminus V(C) \), then both the following propositions are established:

1. The number of the nonfull internal vertex in \( V(C) \) is at most 2.
2. When the number of nonfull internal vertex in \( V(C) \) is 2, then there is at least one vertex with degree 2 in the two nonfull internal vertices in \( V(C) \).

**Theorem 5.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \). If the only circle in \( T^* \) is \( C \), there is no nonfull internal vertex in the set of \( V(T^*) \setminus V(C) \), and the number of the nonfull internal vertex in the set of \( V(C) \) is equal to or greater than 2, then the length of the circle is 3, that is, \( |V(C)| = 3 \).

**Theorem 6.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \), if \( C \) is the only circle in \( T^* \), then \( |V(C)| = 3 \).

**Theorem 7.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \), and let \( r \) be the vertex that corresponds to a maximum component in the component of the Perron vector of \( T^* \). \( T^* \) is the rooted unicyclic graph with root node \( r \), let \( C = \{r, g_1, g_2\} \). Let \( d(u, v) \) be the shortest distance between vertex \( u \) and vertex \( v \) in \( T^* \), denote that \( W_1 = \{|i| \text{ is the leaf node of } T^*, \text{ and the shortest path from } i \text{ to } r \text{ neither pass } g_1 \text{ nor pass } g_2; \} W_2 = \{|i| \text{ is the leaf node of } T^*, \text{ and the shortest path from } i \text{ to } r \text{ either pass } g_1 \text{ or pass } g_2; \} \), then the following propositions are established:

1. If \( W_2 = \emptyset \), then \( \max_{i \in W_1} d(i, r) = 1 \).
2. If \( d(g_1) = 2 \), then for the arbitrary leaf node \( i \) in \( T^* \), we all have \( \{1 - d(i, r)\} \leq 1 \).
3. If \( d(g_2) = 2 \), then for the arbitrary leaf node \( i \) in \( T^* \), we all have \( \{1 - d(i, r)\} \leq 1 \).
4. If \( W_2 \neq \emptyset \), then \( \min_{i \in W_2} d(i, r) \geq \max_{i \in W_1} d(i, r) \).

**Theorem 8.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \), \( x = (x_1, x_2, \ldots, x_n)^T \) is the Perron vector of \( T^* \), \( r \) is the vertex that corresponds to a maximum component in the component of the Perron vector of \( T^* \). Let \( T^* \) be the rooted unicyclic graph with root node \( r \), then \( T^* \) is an almost full-degree unicyclic graph with root node \( r \).

**Theorem 9.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \), \( x = (x_1, x_2, \ldots, x_n)^T \) is the Perron vector of \( T^* \), \( r \) is the vertex that corresponds to a maximum component in the component of the Perron vector of \( T^* \), and \( T^* \) is the rooted unicyclic graph with root node \( r \), \( T^* \) has only one nonfull internal vertex \( u \). Suppose that \( C \) is the only one circle in \( T^* \), and \( V(C) = \{r, g_1, g_2\} \), denote that \( W_1 = \{|i| \text{ is the leaf node of } T^*, \text{ and the shortest path from } i \text{ to } r \text{ neither pass } g_1 \text{ nor pass } g_2; \} W_2 = \{|i| \text{ is the leaf node of } T^*, \text{ and the shortest path from } i \text{ to } r \text{ either pass } g_1 \text{ or pass } g_2; \} \). Assume that \( T^* \neq T_n^\Delta \), that is, \( W_2 \neq \emptyset \), then the following propositions are established:

1. If the distances from all leaves of \( T^* \) to \( r \) are all equal, then there exists a leaf node \( i \) in \( W_1 \) which makes \( (u, i) \) is a pendant edge.
2. If there are two leaves \( i, j \) in \( T^* \) which make \( d(i, r) \neq d(j, r) \) and \( \max_{i \in W_2} d(i, r) = \min_{i \in W_1} d(i, r) \), then either there exists a leaf node \( j_1 \in W_2 \), which makes \( (u, j_1) \) is a pendant edge or \( u \in V(C) \) and \( d(u) = 2 \).
3. If \( \max_{i \in W_2} d(i, r) \neq \min_{i \in W_1} d(i, r) \), then there exists a leaf node \( j_1 \in W_1 \), which makes \( (u, j_1) \) is a pendant edge.

Finally, we obtain the main result of this paper in the following theorem.

**Theorem 10.** Suppose that \( T^* \in T_n^\Delta \), and \( T^* \) is a rooted unicyclic graph with root vertex which is the vertex that corresponds to a maximum component in the component of the Perron vector of \( T^* \), then \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^\Delta \) if and only if \( T^* \equiv H_n^\Delta \).
That is, we describe the structure of the maximal-adjacency-spectrum unicyclic graphs in $T^n_m$. In addition, we give a new upper bound on the adjacency spectral radius of unicyclic graphs on the basis of Theorem 10.

In the following discussion of this paper, we assume that $\Delta$ the maximum degree of unicyclic graphs satisfies $\Delta \geq 3$.

2. Preliminaries

2.1. Some Basic Concepts. A rooted unicyclic graph is a simple nonlinear structure. Figure 1 shows a rooted unicyclic graph with root node $R$.

We can divide a rooted unicyclic graph into levels according to the following principles.

The root nodes are in the first level. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, $R$ is in the first level. In a rooted unicyclic graph, the level which arbitrary vertex is defined as the shortest distance from the vertex to the root node adds 1; for instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, the vertices $A, C, D, E$ are in the second level, the vertices $B, F, G, J, K, L, M, N, O, P, Q$ are in the third level, and the vertices $H, I, V, S$ are in the fourth level. The levels of a rooted unicyclic graph are defined as the maximum of the levels of all the vertices in the rooted unicyclic graph. For instance, the level of the rooted unicyclic graph shown in Figure 1 is 4.

Assume that $T$ is a rooted unicyclic graph, $R$ is the root node of $T$ and $u$ is an arbitrary vertex which is not equal to $R$ in $T$. Suppose that the shortest path from $u$ to $R$ is $u, u_1, u_2, \ldots, u_k$, where $u_1 = u, k \geq 2, u_k = R$, then we call $u_1$ is a father vertex of $u$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, the shortest path from vertex $P$ to vertex $R$ is FAR, $A$ is a father vertex of $R$. The shortest paths from vertex $B$ to vertex $R$ are BAR and BCR, respectively; therefore, $A$ and $C$ are both father vertices of $B$.

Let $T$ be a rooted unicyclic graph, if $u$ and $v$ are two different vertices of $T$, and $u, v$ have the same father vertex, then $u$ is called a brother of $v$. If $w_1$ and $w_2$ are two different vertices in the same level in $T$, and the father vertex of $w_i$ is not equal to the father vertex of $w_j$, then $w_1$ is called a cousin of $w_2$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, vertex $L \neq M, L,$ and $M$ have the same father vertex $D$; therefore, $L$ is a brother of $M$. Besides, vertices $L, Q$ are two vertices in the same level in $T$, and the father vertex of $L$ is not equal to the father vertex of $Q$; therefore, $L$ is a cousin of $Q$.

The vertices (except $u$) on the shortest path that connects the root node to vertex $u$ are called the direct ancestor of the vertex $u$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, the shortest path from the root node $R$ to the vertex $M$ is $RDM$; therefore, $R$ and $D$ are both the direct ancestors of $M$.

Assume that $u$ and $v$ are two different vertices in the rooted unicyclic graph $T$, the level of the vertex $u$ in $T$ is $k_1$, and the level of the vertex $v$ in $T$ is $k_2$, where $k_2 < k_1$ and $v$ is not the direct ancestor of $u$, then we call $v$ is a collateral ancestor of $u$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, the level of vertex $L$ in $T$ is 3, the level of vertex $E$ in $T$ is 2, and $E$ is not the direct ancestor of $L$; therefore, vertex $E$ is the collateral ancestor of vertex $L$.

Suppose that $T$ is a rooted unicyclic graph, if vertex $v$ and vertex $w$ are both direct ancestors of vertex $u$, and the level of vertex $v$ in $T$ is larger than the level of vertex $w$ in $T$, then the generation of vertex $v$ to $u$ is closer than the generation of vertex $w$ to vertex $u$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, the shortest path from vertex $R$ to vertex $Q$ is REQ, vertices $R$ and $E$ are both direct ancestors of $Q$, the root node $R$ is in the first level, and vertex $E$ is in the second level; therefore, the generation of vertex $E$ to $Q$ is closer than the generation of vertex $R$ to vertex $Q$.

If $m \geq 2$, and for any number $i$ which satisfies $1 \leq i \leq m$, we all have that $p$ is a direct ancestor of $u_i$, then $p$ is called a common direct ancestor of $u_1, u_2, \ldots, u_m$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, $E$ is both the direct ancestor of $O$ and the direct ancestor of $S$; therefore, $E$ is a common direct ancestor of $O$ and $S$.

If $m \geq 2$, $p$ is a common direct ancestor of $u_1, u_2, \ldots, u_m,$ and $q$ which is the arbitrary direct ancestor of $u_1, u_2, \ldots, u_m$, satisfies that $q$ is either equal to $p$ or the direct ancestor of $p$, then $p$ is called the common direct ancestor of $u_1, u_2, \ldots, u_m$ of the nearest generation. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, $A$ is the common direct ancestor of $F, I$ of the nearest generation.

Let $u, v$ be two cousins of $u$, if the common direct ancestor of $u$ and $w$ of the nearest generation is the common direct ancestor of $u$ and $v$ of the nearest generation, then $v$ is the cousin of $u$ with generation closer than $w$. For instance, in the rooted unicyclic graph with root node $R$ shown in Figure 1, $H$ and $S$ are two cousins of $V$, and the common direct ancestor of $V$ and $H$ of the nearest generation is $A$, the common direct ancestor of $V$ and $S$ of the nearest generation is $R$, and $R$ is the ancestor of $A$; therefore, $H$ is the cousin of $V$ generation closer than $S$.

In order to give the main results of this paper, we introduce some basic definitions and lemmas.

2.2. Some Definitions

Definition 1. Suppose that $T^\ast \in T^n_m$, if for any $T \in T^n_m$ all have that $\rho(T) \leq \rho(T^\ast)$ establish, then $T^\ast$ is called a maximal-adjacency-spectrum unicyclic graph in $T^n_m$.
Definition 2. Suppose that \( k \geq 2 \) and \( v_0, v_1, \ldots, v_k \) are vertices different from each other in graph \( T \), if \( d(v_0) \geq 3, d(v_k) \geq 3 \), and for any natural number \( i \) which satisfies \( 1 \leq i \leq k - 1 \) all have \( d(v_i) = 2 \), then \( v_0, v_1, \ldots, v_k (k \geq 2) \) a path of graph \( T \) is called an internal path of graph \( T \).

Definition 3. Suppose that \( T = (V, E) \) is a unicyclic graph, and the degree of \( T \) is \( \Delta (\Delta \geq 3) \), \( v \in V \) is called a nonfull vertex of \( T \), which means \( v \) satisfies \( 2 \leq d(v) < \Delta \).

Definition 4. Suppose that \( T = (V, E) \) is a simple connected graph with \( n \) vertices, the vertices in \( T \) with degree 1 are called the pendant point of \( T \), or call that vertex in the leaf node of \( T \); for convenience, the leaf node of \( T \) is sometimes simply called leaf node of \( T \). The edge associated with the pendant point is called pendant edge.

Definition 5. Suppose that \( T = (V, E) \) is a unicyclic graph, and the maximum degree of \( T \) is \( \Delta (\Delta \geq 3) \), if \( T \) satisfies or \( T \equiv T_{\Delta}^{n,2} \), where \( T_{\Delta}^{n,2} \) is shown in Figure 2, and \( r \) is the root node of \( T_{\Delta}^{n,2} \). Or \( T \) is a rooted unicyclic graph with levels more than two, and \( T \) satisfies the following properties:

1. The vertex in the first level is \( r \), and \( r \) is the root node of \( T \); the vertices in the second level from left to right are \( v_1, v_2, \ldots, v_\Delta \).
2. Suppose that the only circle in \( T \) is \( C \), and \( V(C) = \{r, v_1, v_2\} \).
3. The internal vertices of \( T \) are all full-degree vertices.
4. The distance from all the leaf node nodes of \( T \) to \( r \) is equal.

Then, \( T \) is called a completely full \( \Delta \) degree unicyclic graph.

Definition 6. Suppose \( T = (V, E) \) is a unicyclic graph, and the maximum degree of \( T \) is \( \Delta (\Delta \geq 3) \), if \( T \) satisfies or that \( T \equiv T_{\Delta}^{n,2} \), where \( T_{\Delta}^{n,2} \) is shown in Figure 2, and \( r \) is the root node of \( T_{\Delta}^{n,2} \). Or \( T \) is a completely full \( \Delta \) degree unicyclic graph with levels more than two. Or \( T \) is a rooted unicyclic graph obtained from another completely full \( \Delta \) degree unicyclic graph with levels more than two by deleting some right leaf nodes. Then, \( T \) is called an almost completely full \( \Delta \) degree unicyclic graph. We denote the almost completely full \( \Delta \) degree unicyclic graph with \( n \) vertices and maximum degree \( \Delta \) by \( H_{n,\Delta} \).

Definition 7. Suppose that \( T = (V, E) \) is a unicyclic graph, and the maximum of \( T \) is \( \Delta (\Delta \geq 3) \), if \( T \) satisfies or that \( T \equiv T_{\Delta}^{n,3} \), where \( T_{\Delta}^{n,3} \) is shown in Figure 2, and \( r \) is the root node of \( T_{\Delta}^{n,3} \). Or \( T^* \equiv T_{\Delta}^{n,3} \), where \( T_{\Delta}^{n,3} = (V(T_{\Delta}^{n,3}), E(T_{\Delta}^{n,3})) \), \( V(T_{\Delta}^{n,3}) = \{r, v_1, v_2, \ldots, v_\Delta, w_1, w_2, \ldots, w_s\} \) (where \( s \) is the number which satisfies that \( s + 2 \leq \Delta \)), \( E(T_{\Delta}^{n,3}) = \{(r, v_1), (r, v_2), (v_1, v_2), (v_1, v_3), \ldots, (v_1, v_\Delta), \ldots, (v_i, v_j)\} \), and \( r \) is the root node of \( T_{\Delta}^{n,3} \). Or \( T \) is a rooted unicyclic graph with \( k \) levels, and \( T \) satisfies the following properties:

1. \( k \geq 3 \).

2.3. Some Lemmas. Now, we give some lemmas which we use to proof the main results.

Lemma 1 (see [13]). Suppose that \( T \) is a simple connected graph with \( n \) vertices and maximum degree \( \Delta \), \( x = (x_1, x_2, \ldots, x_n)^T \) is the Perron vector of \( T \), \( x_u \) and \( x_v \) correspond to vertices \( u \) and \( v \), respectively, and \( x_u \geq x_v \). If \( w \in N_T(v) \setminus u \), let \( T_1 = T - (v, u) + (u, w) \), if \( T_1 \) is still a simple connected graph, then \( \rho(T_1) > \rho(T) \).
Lemma 2 (see [13]). Suppose that $T$ is a simple connected graph with $n$ vertices and maximum $\Delta$, $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T$, $x_u$ and $x_v$ correspond to vertices $u$ and $v$, respectively, and $x_u \geq x_v$. Suppose that $w_1 \in N_T(v) \setminus u, w_2 \in N_T(V) \setminus u, \ldots, w_k \in N_T(v) \setminus u$. Let $T_1 = T - (v, w_1) - (v, w_2) - \cdots - (v, w_k) + (u, w_1) + (u, w_2) + \cdots + (u, w_k)$. $T_1$ and $T$ are shown in Figure 4. If $T_1$ is still a simple connected graph, then $\rho(T_1) > \rho(T)$.

Lemma 3 (see [13]). Suppose that $T = (V, E)$ is a simple connected graph with $n$ vertices and maximum $\Delta$, $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T$, and suppose that $x_u, x_u, x_v, x_v$ correspond to the four different vertices $u_1, u_2, v_1, v_2$, respectively, where $(u_1, u_2) \in E, (v_1, v_2) \in E$, and $x_u \geq x_u, x_u < x_v$. Let $T_1 = T - (u_1, v_2) - (v_2, v_1) + (u_1, v_1) + (v_2, v_1)$, $T_1$ and $T$ are shown in Figure 5; if $T_1$ is still a simple connected graph, then $\rho(T_1) > \rho(T)$.

Lemma 4 (see [14]). Suppose that $T = (V, E)$ is a simple connected graph, and $v_0v_1 \cdots v_k (k \geq 2)$ is an internal path of $T$. If $T_1 = (V, E)$, $T_1 - v_i v_{i+1} + v_i v_{i+1}$, where $1 \leq i \leq k - 1$, then $\rho(T_1) > \rho(T)$.

Lemma 5 (see [13]). Suppose that $T = (V(T), E(T))$ is a connected graph, if $u \in V(T)$ and $v \notin V(T)$, let $T_1 = T + (u, v)$, then $\rho(T_1) > \rho(T)$.

Lemma 6. Assume that $T \in T_n^\Delta$, the edge set of $T$ is $E(T)$, and $C$ is the only circle in $T$. Suppose that $V(C) = \{u_1, u_2, \ldots, u_l\}$, where $l \geq 4$, and for any natural number $i$ which satisfies $1 \leq i \leq k - 1$, we all have $(u_i, u_{i+1}) \in E(T), (u_i, u_{i-1}) \in E(T)$, denote $u_1 = u_l, u_{i+1} = u_{i-1}, u_{i+2} = u_i, u_{i+3} = u_i$. Suppose that $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T, r_1, r_2, \ldots, r_k$ (where $1 \leq k \leq l - 1$) is the set which consists of all the vertices whose components of Perron vector are equal to $\max_{1 \leq j \leq l} x_u$ in $C$, if for any arbitrary natural number $j$ which satisfies $1 \leq j \leq l + 1$, we all have $\{u_{i,j-1}, u_{i,j+1}, u_{i,j+2}, u_{i,j+3}\} \notin \{r_1, r_2, \ldots, r_k\}$, then there exists $T_1 \in T_n^\Delta$ which makes that $\rho(T_1) > \rho(T)$ holds.

Proof. Since for any arbitrary natural number $j$ which satisfies $1 \leq j \leq l + 1$, we all have $\{u_{i,j-1}, u_{i,j+1}, u_{i,j+2}, u_{i,j+3}\} \notin \{r_1, r_2, \ldots, r_k\}$, we can get $k \geq 2$. Without loss of generality, we assume that $r_1, r_2, \ldots, r_k$ have clockwise arrangement in $C$, as shown in Figure 6, and denote $r_{k+1} = r_1$.

Since for any natural number $j$ which satisfies $1 \leq j \leq l + 1$, we all have $\{u_{i,j-1}, u_{i,j+1}, u_{i,j+2}, u_{i,j+3}\} \notin \{r_1, r_2, \ldots, r_k\}$. We know that there exist two vertices $v_1$ and $v_2$ in $C$ and exist two numbers $i$ and $s$ which satisfy both $1 \leq i \leq k - 1, 1 \leq s \leq k, i < s$, which make $v_1$ is in clockwise arrangement between $r_1$ and $r_{i+1}$, $v_1$ is adjacent to $r_i$, and $v_2$ is in clockwise arrangement between $r_1$ and $r_{s+1}$, $v_2$ is adjacent to $r_s$, and $x_{v_2} \neq \max_{1 \leq j \leq l} x_{u_j}$ and $x_{v_2} \neq \max_{1 \leq j \leq l} x_{u_j}$. From the definition of $r_1, r_2, \ldots, r_k$, we know $x_{v_1} = x_{v_2} > \max(x_{v_1}, x_{v_2})$. Let $T_1 = T - (v_1, v_2) - (r_s, v_2) + (r_s, v_1) + (v_1, v_2)$, then it is easy to know that $T_1 \in T_n^\Delta$. From $x_{v_1} > x_{v_2}$ and $x_{v_1} > x_{v_2}$, by Lemma 3, we have $\rho(T_1) > \rho(T)$; therefore, Lemma 6 holds.

Lemma 7. Assume that $T \in T_n^\Delta, T = (V(T), E(T)), v_{i_1}, v_{i_2}, v_{i_3}$, and $v_4$ are four different vertices of $T$, and $(v_{i_1}, v_{i_2}) \in E(T), (v_{i_2}, v_{i_3}) \in E(T), (v_{i_3}, v_4) \in E(T), x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T, x_{v_1}, x_{v_2}, x_{v_3}, x_{v_4}$, and $x_{v_4}$ correspond to vertices $v_1, v_2, v_3, v_4$, respectively, and $x_{v_4} > x_{v_1} > x_{v_2} > x_{v_3}$. Let $T_1 = T - (v_1, v_2) - (v_2, v_3) + (v_1, v_3) + (v_3, v_4)$, if $T_1$ is still a simple connected graph, then $\rho(T_1) > \rho(T)$. 
3. The Properties and Structure of the Maximal-Adjacency-Spectrum Unicyclic Graphs in $T_n^\Delta$

3.1. The Properties of the Maximal-Adjacency-Spectrum Unicyclic Graphs in $T_n^\Delta$

First, we give the properties of the Perron vector of the maximal-adjacency-spectrum unicyclic graphs in $T_n^\Delta$, as in the following theorems:

**Theorem 11.** Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$ if $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T^*$ such that $x^\ast_\nu = \max_{1\leq i\leq n} x_i$ and $d(v^\ast) < \Delta$. Denote $p = d(v^\ast)$, it is obvious that $p \geq 2$; hence, $2 \leq p < \Delta$. We choose a vertex $u$ with degree $\Delta$ in $V(T^*)$, suppose that $N_{T^*}(u) = \{v_1, v_2, \ldots, v_p\}$. For $T^*$ is a unicyclic graph, it is easy to know that there are $\Delta - p$ vertices $v_{j_1}, v_{j_2}, \ldots, v_{j_{\Delta - p}}$ in the set of $N_{T^*}(u) \backslash N_{T^*}(v^\ast)$ such that $T^* - (u, v_{j_1}) - (u, v_{j_2}) - \cdots - (u, v_{j_{\Delta - p}}) + (v^\ast, v_{j_1}) + (v^\ast, v_{j_2}) + \cdots + (v^\ast, v_{j_{\Delta - p}})$ is still a simple connected graph.

Denote $T_1 = T^* - (u, v_{j_1}) - (u, v_{j_2}) - \cdots - (u, v_{j_{\Delta - p}}) + (v^\ast, v_{j_1}) + (v^\ast, v_{j_2}) + \cdots + (v^\ast, v_{j_{\Delta - p}})$, then it is easy to know $T_1 \in T_n^\Delta$. Again by $x^\ast \geq x^\ast_\nu$, by Lemma 2, we get $\rho(T_1) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, hence, the hypothesis is not established; therefore, Theorem 11 holds.

**Theorem 12.** Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, and the only circle in $T^*$ is $C$, $x = (x_1, x_2, \ldots, x^\ast, \ldots, x_{n^2})^T$ is the Perron vector of $T^*$, if the component $x^\ast_\nu$ which corresponds to the vertex $u^\ast$ in $x$ satisfies that $x^\ast_\nu = \max_{1\leq i\leq n^2} x^\ast_i$, then $u^\ast \in V(C)$.

**Proof.** Assume that the proposition is not established, we suppose that there exists a vertex $u^\ast$ in $T^*$ such that $x^\ast_\nu = \max_{1\leq i\leq n^2} x^\ast_i$ and $u^\ast \in V(T^*) \setminus V(C)$. From $x^\ast_\nu = \max_{1\leq i\leq n^2} x^\ast_i$ and Theorem 11, we get $d(u^\ast) = \Delta$. For $d(u^\ast) = \Delta$, $u^\ast \in V(T^*) \setminus V(C)$ and $T^*$ is a unicyclic graph, we know that there exists a path $u^\ast u_1 u_2 \cdots u_k (k \geq 1)$ whose length is $k$ in $T^*$, which makes $u^\ast \notin V(C), u_i \notin V(C), \ldots, u_k \notin V(C), u_1, u_2, \ldots, u_k$ are difference with each other, and $u_k$ is the leaf node.

First, for $\forall v \in V(C)$, we have $x^\ast_i > x^\ast_{uk}$. Otherwise, suppose there exists a vertex $v^\ast$ in $V(C)$ such that $x^\ast_i \leq x^\ast_{uk}$. Now according to the value of $d(v^\ast)$, we discuss the following two cases:

Case 1. $d(v^\ast) < \Delta$.

Since $v^\ast \in V(C)$, we have $|N_{T^*}(v^\ast)| \geq 2$; thus in the set of $V(T^*)$, there exists a vertex $v_1$ which satisfies $x^\ast_i \in N_{T^*}(v^\ast)$ such that $T^* - (v^\ast, v_1) + (v_1, v_2) + \cdots + (v_1, v_p)$ is still a simple connected graph. Denote $T_2 = T^* - (v^\ast, v_1) + (v_1, v_2) + \cdots + (v_1, v_p)$, it is easy to know $T_2 \in T_n^\Delta$. By Lemma 1, we get $\rho(T_2) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

Case 2. $d(v^\ast) = \Delta$.

In this case, it is easy to know that in the set of $N_{T^*}(v^\ast)$, there exist $\Delta - 1$ vertices $v_2, v_3, \ldots, v_p$ such that $T^* - (v^\ast, v_2) - (v_2, v_3) - \cdots - (v_2, v_p) + (v_3, v_2) + \cdots + (v_p, v_2)$ is still a simple connected graph. Denote $T_3 = T^* - (v^\ast, v_2) - (v_2, v_3) - \cdots - (v_2, v_p) + (u_k, v_2) + (u_k, v_3) + \cdots + (u_k, v_p)$, then it is easy to know $T_3 \in T_n^\Delta$. From $x^\ast_i \leq x^\ast_{u_k}$ by Lemma 2, we can get $\rho(T_3) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

From the above discussion of the two cases, we know that the hypothesis is not established. Hence, for $\forall v \in V(C)$, we all have that $x^\ast_i > x^\ast_{uk}$ holds.

Second, denote $u^\ast$ by $u_0$, suppose that $v$ is the vertex which is nearest to $u^\ast$ in $C$. Choose two vertices $v_1$ and $v_2$ different from $v$ in $C$, then $x^\ast_i \geq x_{u_1}, x_{u_2} \geq x^\ast_i, v_1 > x_{u_1}$ and $x^\ast_i > x_{u_2}$. Thus, we have that there exists a natural number $l$ which satisfies $1 \leq l \leq k$ such that at least one of the following two inequality groups: $\{1\} x^\ast_i \geq x^\ast_{u_1}, x_{u_2} > x_{u_1}$ and $\{2\} x^\ast_i \geq x_{u_1}, x^\ast_i > x_{u_2}$. Without loss of generality, we assume that there exists a natural number $l$ which satisfies $1 \leq l \leq k$ such that $x^\ast_i \geq x^\ast_{u_1}, x_{u_2} > x_{u_1}$. Then, let $T_2 = T^* - (u_1, u_2) - (v^\ast, v_1) + (v_1, u_2) + (v_1, u_1) - (v^\ast, u_1)$, then it is easy to know $T_2 \in T_n^\Delta$. By Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$. Therefore, Theorem 12 holds.
Lemma 8. Assume that $T \in T_n^3$, $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T$, and $C$ is the only circle in $T$, $V(C) = \{u_1, u_2, \ldots, u_l\}$, suppose that $x_{u_1}, x_{u_2}, \ldots, x_{u_l}$ corresponds to the vertices $u_1, u_2, \ldots, u_l$ respectively. If $l \geq 4$, and $x_u = x_{u_1} = \cdots = x_{u_l}$, then there must exist $T_1 \in T_n^3$ such that $\rho(T_1) > \rho(T)$.

Proof. Assume that the proposition is not established, then $T$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$. From Theorem 12, we can get $x_{u_i} = x_{u_j} = \cdots = x_v = max_{1 \leq i \leq n} x_i$; again by Theorem 11, we have $d(u_i) = d(u_j) = \cdots = d(u_l) = \Delta \geq 3$; hence, for any natural number $i$ which satisfies $1 \leq i \leq l$, and we all have $N_T(u_i) \cap V(C) \neq \emptyset$. Besides, from Theorem 12, we get that for $\forall v \in V(T) \cap V(C)$, we all have $x_v < max_{1 \leq i \leq n} x_i$.

Without loss of generality, we assume that $u_1, u_2, \ldots, u_l$ have clockwise arrangement in $C$. Since $N_T(u_i) \cap V(C) \neq \emptyset$, choose $v \in N_T(u_i) \cap V(C)$, then we have $x_v < x_{u_i}$. For $l \geq 4$, we can know $u_i, v, u_{i-1}$ and $u_{i+1}$ are different from each other. From $x_{u_i} = x_{u_{i-1}} = \cdots = x_{u_1}$ and $x_v > x_{u_l}$, we know that $x_{u_{l-1}} > x_l > x_v > x_{u_l} > x_{u_l}$. Let $T_1 = T - (u_{l-1}, v) - (u_{l-1}, u_l) - (u_1, u_{i-1}) + (u_1, u_{i-1}) + (v_1, v)$, then it is easy to know $T_1 \in T_n^3$. From $x_{u_{l-1}} > x_{u_1}$ and $x_v > x_{u_l}$, by Lemma 3, we have that $\rho(T_1) > \rho(T)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$. Therefore, Lemma 8 holds.

Lemma 9. Assume that $T \in T_n^3$, where $T = (V(T), E(T))$, $C$ is the circle of $T$, $V(C) = \{u_1, u_2, \ldots, u_l\}$, for any natural number $i$ which satisfies $1 \leq i \leq l - 1$, we all have $(u_i, u_{i-1}) \in E(T)$, $(u_i, u_{i+1}) \in E(T)$. If there exists a natural number $i_0$ which satisfies $1 \leq i_0 \leq l$ such that $d(u_{i_0}) = 2$, then there exists $T_1 \in T_n^3$ such that $\rho(T_1) > \rho(T)$.

Proof. Assume that the proposition is not established, then $T$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$.

Form Theorems 11 and 12, we know that there exists a natural number $j$ which satisfies $1 \leq j \leq l$ such that $x_{u_j} = max_{1 \leq i \leq n} x_i$ and $d(u_j) = \Delta \geq 3$. Now, we discuss the following two cases: Case 1. There are at least two vertices with the degree not less than 3 in $V(C)$.

Denote $u_{i+1} = u_1$, for any natural number $i$ which satisfies $1 \leq i \leq l - 1$, we all have $(u_i, u_{i+1}) \in E(T)$ and $(u_i, u_l) \in E(T)$; hence, for any natural number $i$ which satisfies $1 \leq i \leq l$, we all have $(u_i, u_{i+1}) \in E(T)$ and $(u_i, u_l) \in E(T)$. And for there exists a natural number $i_0$ which satisfies $1 \leq i_0 \leq l$ such that $d(u_{i_0}) = 2$ and there are at least two vertices with the degree not less than 3 in $V(C)$, then we know that there exist two natural numbers $t$ and $m$ which satisfy $m \geq 2$ and $1 \leq t \leq l$ such that $u_t u_{t+1} \cdots u_{t+m}$ is an internal path. Let $T_1 = (V(T_1), E(T_1))$, where $V(T_1) = V(T) \setminus \{u_{i_0}\}$ and $E(T_1) = E(T) - (u_{i_0}, u_{i_0+1}) - (u_{i_0+m}, u_{i_0+m+1}) + (u_{i_0+m}, u_{i_0+1})$. It is easy to know $T_1 \in T_n^3$ and by Lemma 4, we have that $\rho(T_1) > \rho(T)$ holds.

Suppose that $v_1$ is an arbitrary leaf node of $T_1$. Let $T_2 = T_1 + (v_1, u_1)$, then it is easy to know $T_2 \in T_n^3$ and by Lemma 5, we have that $\rho(T_2) > \rho(T_1)$ holds, and thus, $\rho(T_2) > \rho(T)$. Therefore, this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$.

Case 2. There is only one vertex with degree not less than 3 in $V(C)$.

In this case, it is easy to know that the only one vertex with degree not less than 3 must be $u_j$. Suppose that $V(C) = \{v_1, v_2, \ldots, v_{l-1}, u_1\}$ and $v_1, v_2, \ldots, v_{l-1}, u_j$ have clockwise arrangement in $C$, as shown in Figure 7. From Theorems 11 and 12, we get $x_{u_j} > max\{x_v, x_{v_j}, x_{v_{j+1}}, \ldots, x_{v_{l-1}}\}$. From $l \geq 4$, we can know $v_{l-1}, v_{l-2}$ and $v_1$ are different. And for $x_{u_j} > x_{v_{l-2}}$, it is easy to prove that $x_{v_{l-2}} > x_{v_{l-3}}$ holds. Otherwise, $x_{v_1} \leq x_{v_{l-3}}$.

Let $T_1 = T - (v_{l-1}, v_{l-2}) - (u_{j}, v_1) + (u_j, v_{l-2}) + (v_1, v_{l-2})$, then it is easy to know $T_1 \in T_n^3$. From $x_{v_{l-1}} > x_{v_{l-2}}$ and $x_{v_{l-2}} > x_{u_1}$, by Lemma 3, we have that $\rho(T_1) > \rho(T)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$; hence, $x_{u_j} > x_{v_{l-2}}$. Let $T_2 = T - (v_{l-1}, v_{l-2}) + (v_{l-1}, v_1)$, then it is easy to know $T_2 \in T_n^3$, and by Lemma 1, we have that $\rho(T_2) > \rho(T)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$.

By consideration of the above two cases, we know that the hypothesis is not established. Therefore, Lemma 9 holds.

Lemma 10. Assume that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$, and $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T^*$. Then, for any leaf node $i$ and any vertex $j$ which is not the leaf node in $T^*$, we all have that $x_i < x_j$, where $x_i$ and $x_j$ correspond to the vertices $i$ and $j$, respectively.

Proof. Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^3$, and $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T^*$. Let $j_0$ be any one of the vertices whose component is equal to $max_{1 \leq i \leq n} x_i$ in $x$, then from Theorem 11, we know $d(j_0) = \Delta$. Then, for any nonleaf node $u$ which is not $j_0$ in $T^*$, and for the arbitrary leaf node $i$ in $T^*$, we all have that $x_i \geq x_j$ holds. Otherwise, there exists a vertex $w$ which is not the vertex $j_0$ and is not a leaf node $i$ in $T^*$, which makes $x_w < x_i$. For $w$ is not the leaf node, hence $d(w) > 2$, thus there exists a vertex $v$ in the set of $N_T(w)$ such that $T^* - (v, w) + (v, i)$ still belong to $T_n^3$. Let
For the properties of the nonfull internal vertices of the maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, we have the following theorems.

**Theorem 13.** Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, if the only circle in $T^*$ is $C$, and there exists a nonfull internal vertex in the set of $V(T^*) \setminus V(C)$, then the number of all the nonfull internal vertices of $T^*$ is one.

**Proof.** Assume that the proposition is not established, then suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, the only circle in $T^*$ is $C$, there exists a nonfull internal vertex in the set of $V(T^*) \setminus V(C)$, and the number of the nonfull internal vertex in $T^*$ is more than 1. Without loss of generality, assume that $u_1$ and $u_2$ are two nonfull internal vertices in $T^*$, where $u_i \in V(T^*) \setminus V(C)$.

Let $x = (x_1, x_2, \ldots, x_n)^T$ be the Perron vector of $T^*$, $u_1$ and $u_2$ correspond to the vertices $u_1$ and $u_2$, respectively. Now according to whether $u_1$ and $u_2$ adjacent or not, we discuss the following two cases:

Case 1. $u_1$ and $u_2$ adjacent.

For case 1, we discuss the following two subcases again according to the value of $x_{u_1}$ and $x_{u_2}$.

Subcase 1. $x_{u_1} \geq x_{u_2}$.

Since $u_2$ is the nonfull internal vertex in $T^*$, then $N_{T^*}(u_2) \neq \emptyset$, choose $u \in N_{T^*}(u_2) \setminus u_1$. Let $T_1 = T^* - (u, u_2) + (w, u_1)$, then it is easy to know $T_1 \in T_n^\Delta$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$, this holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

Subcase 2. $x_{u_1} < x_{u_2}$.

Since $u_1$ is the nonfull internal vertex in $T^*$, then $N_{T^*}(u_1) \setminus u_2 \neq \emptyset$, choose $u \in N_{T^*}(u_1) \setminus u_2$. Let $T_1 = T^* - (w, u_1) + (w, u_2)$, then it is easy to know $T_1 \in T_n^\Delta$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$, this holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

Case 2. $u_1$ and $u_2$ are not adjacent.

Since $u_1$ and $u_2$ are the nonfull internal vertices in $T^*$, we have that $|N_{T^*}(u_1) \setminus N_{T^*}(u_2)| \geq 1$ and $|N_{T^*}(u_2) \setminus N_{T^*}(u_1)| \geq 1$ hold at the same time. For case 2, we discuss the following two subcases again according to the value of $x_{u_1}$ and $x_{u_2}$.

Subcase 1. $x_{u_1} \leq x_{u_2}$.

Since $|N_{T^*}(u_1) \setminus N_{T^*}(u_2)| \geq 1$ and $T^*$ is a unicyclic graph, we know that there exists $w \in N_{T^*}(u_1) \setminus N_{T^*}(u_2)$ such that $T^* - (w, u_1) + (w, u_2)$ is still a simple connected graph. Denote $T_1 = T^* - (w, u_1) + (w, u_2)$, then it is easy to know $T_1 \in T_n^\Delta$; by Lemma 1, we have that $\rho(T_1) > \rho(T^*)$, holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

Subcase 2. $x_{u_1} > x_{u_2}$.

For $|N_{T^*}(u_2) \setminus N_{T^*}(u_1)| \geq 1$ and $T^*$ is a unicyclic graph, we know that there exists $w \in N_{T^*}(u_2) \setminus N_{T^*}(u_1)$ such that $T^* - (w, u_2) + (w, u_1)$ is still a simple connected graph. Denote $T_1 = T^* - (w, u_2) + (w, u_1)$, then it is easy to know $T_1 \in T_n^\Delta$; by Lemma 1, we have that $\rho(T_1) > \rho(T^*)$, holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

Hence, from the discussions of case 1 and case 2, we can know that the hypothesis is not established; therefore, Theorem 13 holds.

**Theorem 14.** Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, let $C$ be the only circle in $T^*$, and $|V(C)| = 3$, if there is no nonfull internal vertex in the set of $V(T^*) \setminus V(C)$, then both the following propositions are established:

1. The number of the nonfull internal vertex in $V(C)$ is at most 2.

2. When the number of nonfull internal vertex in $V(C)$ is 2, then there is at least one vertex with degree 2 in the two nonfull internal vertices in $V(C)$.

**Proof.** Let $x = (x_1, x_2, \ldots, x_n)$ be the Perron vector of $T^*$.

(1) Suppose that a vertex $v$ in $T^*$ satisfies $x_v = \max_{1 \leq i \leq n} x_i$, then from Theorem 12, we get $v \in V(C)$, and from Theorem 11, we know $d(v) = \Delta$. Hence, the number of the nonfull internal vertices in $V(C)$ is at most 2, and then, (1) of Theorem 14 holds.

(2) When the number of nonfull internal vertices in $V(C)$ is 2, without loss of generality, we assume that $u_1$ and $u_2$ are the nonfull internal vertices in $V(C)$. Suppose that $x_{u_1}$ and $x_{u_2}$ correspond to the vertices $u_1$ and $u_2$, respectively. Assume that $d(u_1) \neq 2$ and $d(u_2) \neq 2$, then we must have that $d(u_1) \geq 3$ and $d(u_2) \geq 3$ hold. Hence, $N_{T^*}(u_1) \setminus V(C) \neq \emptyset$ and $N_{T^*}(u_2) \setminus V(C) \neq \emptyset$. Choose $s_1 \in N_{T^*}(u_1) \setminus V(C), s_2 \in N_{T^*}(u_2) \setminus V(C)$. Without loss of generality, we assume that $x_{u_1} \geq x_{u_2}$, and let $T_1 = T^* - (u_2, s_1) + (s_2, u_1)$, then it is easy to know $T_1 \in T_n^\Delta$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$, holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$. Hence, the hypothesis is not established. Therefore, either $d(u_1) = 2$ or $d(u_2) = 2$, then (2) of Theorem 14 holds.

By consideration, Theorem 14 holds.

### 3.2. The Structure of the Maximal-Adjacency-Spectrum Unicyclic Graphs in $T_n^\Delta$

For the length of the circle of the maximal-adjacency-spectrum unicyclic graphs in $T_n^\Delta$, we have the following theorems.
Theorem 15. Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$. If the only circle in $T^*$ is $C$, there is no nonfull internal vertex in the set of $V(T^*)\setminus V(C)$, and the number of the nonfull internal vertex in the set of $V(C)$ is equal to or greater than 2, then the length of the circle is 3, that is, $|V(C)| = 3$.

Proof. Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$, the only circle in $T^*$ is $C$, there is no nonfull internal vertex in the set of $V(T^*)\setminus V(C)$, and the number of the nonfull internal vertices in the set of $V(C)$ is not less than 2. Denote $|V(C)| = m$, and assume that Theorem 15 is not established, then $m \geq 4$. Suppose that $u_1 \in V(C), u_2 \in V(C)$, and $u_1$ and $u_2$ are two different nonfull internal vertices in $T^*$. Let $x$ be the Perron vector of $T^*$, and suppose that $x_v$ and $x_u$ correspond to the vertices $u_1$ and $u_2$. Now according to the value of $m$, we discuss the following two cases:

Case 1. $m \geq 5$.

In case 1, there exists a path $u_1v_1v_2\cdots v_ku_2$ which satisfies $k \geq 2$ in $C$. Without loss of generality, we assume that $x_v \geq x_u$. Let $T_1 = T^* - (v_2, u_2) + (v_1, u_1)$, then it is easy to know $T_1 \in T_n^\alpha$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$.

Case 2. $m = 4$.

Now according to whether the vertices $u_1$ and $u_2$ adjacent or not, we discuss the following two subcases again:

Subcase 1. If $m = 4$ and $u_1$ and $u_2$ are adjacent.

At this time, it is easy to know that there is a path $u_1v_1v_2\cdots v_4u_2$ which satisfies $k \geq 2$ in $C$. Without loss of generality, we assume that $x_v \geq x_u$. Let $T_1 = T^* - (v_2, u_2) + (v_2, u_1)$, then it is easy to know $T_1 \in T_n^\alpha$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$.

Subcase 2. If $m = 4$ and $u_1$ and $u_2$ are not adjacent.

Suppose that $V(C) = \{u_1, u_2, v_1, w_1\}$. First, we must have that $d(v_1) = d(w_1) = 4$ holds; otherwise, there must exist two adjacent nonfull internal vertices in $C$. From the discussion of the subcase 1 in case 2, we know that it will imply a contradiction. Without loss of generality, we assume that the position relationship of the vertices $v_1, w_1, u_1, u_2$ in $C$ is shown in Figure 8.

Second, we must have $d(u_1) \geq 3$ and $d(u_2) \geq 3$. Otherwise, there are at least one of the two inequalities, $d(u_1) < 3$ and $d(u_2) < 3$, holds. Without loss of generality, assume that $d(u_1) < 3$. For $u_1 \in V(C)$, $d(u_1) = 2$. And since $d(v_1) = d(w_1) = 4$ holds, we have that $v_1, u_1$ is an internal path, let $T_1 = (V(T^*), E(T_1))$, where $V(T^*_1) = V(T^*)\setminus\{u_1\}, E(T_1) = E(T^*) - (v_1, u_1) - (u_1, w_1) + (v_1, w_1)$, then it is easy to know $T_1 \in T_n^\alpha$. By Lemma 4, we have that $\rho(T_1) > \rho(T^*)$ holds. Let $w_1$ be an arbitrary leaf node in $T_1$, and let $T_2 = T_1 + (u_1, w_1)$, then it is easy to know $T_2 \in T_n^\alpha$. By Lemma 5, we have that $\rho(T_2) > \rho(T_1)$ holds; hence, $\rho(T_2) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$.

From $d(u_1) \geq 3$ and $d(u_2) \geq 3$, we know that $N_{T^*}(u_1) \setminus V(C) \neq \emptyset$ and $N_{T^*}(u_2) \setminus V(C) \neq \emptyset$. Choose $s_1 \in N_{T^*}(u_1) \setminus V(C)$ and $s_2 \in N_{T^*}(u_2) \setminus V(C)$. Without loss of generality, assume that $x_s \geq x_u$. Let $T_1 = T^* - (s_2, u_2) + (s_2, u_1)$, then it is easy to know $T_3 \in T_n^\alpha$. By Lemma 1, we have that $\rho(T_3) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$.

Hence, from the discussion of case 1 and case 2, we know that $m \geq 4$ does not hold. Therefore, Theorem 15 holds.

Theorem 16. Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$, if $C$ is the only circle in $T^*$, then $|V(C)| = 3$.

Proof. Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$ and $C$ is the only circle in $T^*$. Denote $|V(C)| = k$ assume that Theorem 16 does not hold, then we have $l \geq 4$. From Theorems 13 and 15, we can get that there is at least one nonfull internal vertex in $T^*$. Suppose that $V(C) = \{u_1, u_2, \ldots, u_l\}$, and $x = (x_1, x_2, \ldots, x_l)^T$ is the Perron vector of $T^*$. By Theorem 12, we can get $\max_{1 \leq i \leq l} x_i = max_{1 \leq j \leq n} x_j$. Then, from $l \geq 4$, $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$, and from Lemma 8, we can get $\max_{1 \leq i \leq l} x_i > \min_{1 \leq j \leq n} x_j$. Now, according to the value of $l$, we discuss the following two cases:

Case 1. $l = 4$.

Suppose that $V(C) = \{u_1, u_2, u_3, u_4\}$, from Theorem 12, we have that $\max_{1 \leq i \leq 4} x_i = \max_{1 \leq j \leq n} x_j$ holds. Without loss of generality, assume that $x_{u_4} = \max_{1 \leq i \leq 4} x_i$, then we have $x_u = \max_{1 \leq j \leq n} x_j$; again from Theorem 11, we can get $d(u_4) = \Delta (\Delta \geq 3)$. Without loss of generality, we assume that $u_1, u_2, u_3, u_4$ have antilockwise arrangement in $C$, and the position of the relationship of these vertices is shown in Figure 9.
Figure 9: Cycle C with four vertices.

In the situation of case 1, we could prove that the following six propositions hold. 

**Proposition 1.** For any vertex $u_i$ which satisfies $1 \leq i \leq 4$ in $V(C)$, we all have that $N_{T^*}(u_i) \cap V(C) \neq \emptyset$ holds.

For there is at most one nonfull internal vertex in $T^*$, there is at most one of $d(u_i), d(u_4), \text{and } d(u_3)$ unequal to $\Delta(\geq 3)$. Besides, $\min\{d(u_i), d(u_4), d(u_3)\} \geq 3$; otherwise, $\min\{d(u_i), d(u_4), d(u_3)\} = 2$. Since there is at most one nonfull internal vertex in $T^*$, hence there must exist an internal path $q_1q_2q_3$ in C. Let $T_1 = (V(T_1), E(T_1))$, where $V(T_1) = V(T^*) \setminus \{q_2\}$, $E(T_1) = E(T^*) \setminus (q_1, q_2) - (q_2, q_3)$. Then, it is easy to know that $T_1 \in T_{n-1}$. And by Lemma 4, we have that $\rho(T_1) > \rho(T^*)$ holds. Let $w_1$ be an arbitrary leaf node in $T_1$, and let $T_2 = T_1 + (q_2, w_1)$, then it is easy to know $T_2 \in T_n^*$. By Lemma 5, we have that $\rho(T_2) > \rho(T_1)$ holds. Hence, $\rho(T_2) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^*$. Then, $\min\{d(u_i), d(u_4), d(u_3)\} \geq 3$, and $\min\{d(u_i), d(u_4), d(u_3)\} \geq 3$. Therefore, for any vertex $u_i$ which satisfies $1 \leq i \leq 4$ in the set of $V(C)$, we all have that $N_{T^*}(u_i) \cap V(C) \neq \emptyset$ holds.

**Proposition 2.** $x_{u_i} = \min\{x_{u_{i1}}, x_{u_{i2}}, x_{u_{i3}}\}$.

Assume that $x_{u_i} = \min\{x_{u_{i1}}, x_{u_{i2}}, x_{u_{i3}}\}$ is not established, and we have $x_{u_i} > \max\{x_{u_{i1}}, x_{u_{i2}}, x_{u_{i3}}\}$. Without loss of generality, assume that $\min\{x_{u_{i1}}, x_{u_{i2}}, x_{u_{i3}}\} = x_{u_{i1}}$, then we have $x_{u_i} > x_{u_{i1}}$.

Let $T_1 = T - (u_i, u_4) - (u_3, u_4)$, then it is easy to know $T_1 \in T_n^*$. From $x_{u_i} \geq x_{u_4}$ and $x_{u_4} > x_{u_3}$, by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^*$; hence, the hypothesis is not established. Therefore, $x_{u_i} = \min\{x_{u_{i1}}, x_{u_{i2}}, x_{u_{i3}}\}$.

**Proposition 3.** For $\forall v \in N_{T^*}(u_4) \cap V(C)$, we all have that $x_{u_4} = x_v$ holds.

And for $\forall v \in N_{T^*}(u_4) \cap V(C)$, we all have that $x_w = x_{u_4}$ holds. From Proposition 1, we know $N_{T^*}(u_4) \cap V(C) \neq \emptyset$. Assume that, for $\forall v \in N_{T^*}(u_4) \cap V(C)$, we all have that the proposition $x_{u_4} = x_v$ is not established, then there must exists a vertex $v_2 \in N_{T^*}(u_4) \cap V(C)$ such that $x_{u_2} \neq x_{v_2}$.

**Proposition 4.** $d(u_i) = \Delta$ and $d(u_4) = \Delta$.

If $d(u_i) = \Delta$ is not established, then $d(u_i) < \Delta$. From Proposition 1, we know $N_{T^*}(u_i) \cap V(C) \neq \emptyset$. Choose $v_1 \in N_{T^*}(u_1) \cap V(C)$, and let $T_1 = T^* - (v_1, u_2) + (v_3, u_2)$, then it is easy to know $T_1 \in T_n^*$. From Proposition 2, we know $x_{u_1} \leq x_{u_2}$, and by Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^*$. Hence, the hypothesis is not established, that is, $d(u_4) = \Delta$. The same reason, we can prove that $d(u_i) = \Delta$ holds.

**Proposition 5.** $x_{u_4} = x_{u_2}$ and $x_{u_3} = x_{u_1}$.

Assume that $x_{u_4} \neq x_{u_2}$, then from $x_{u_4} = \max_{1 \leq i \leq 4} x_{u_i}$, we know $x_{u_4} > x_{u_2}$. From Proposition 1, we can get $N_{T^*}(u_4) \cap V(C) \neq \emptyset$. Choose $v_2 \in N_{T^*}(u_4) \cap V(C)$, let $T_1 = T^* - (u_1, u_4) - (u_2, v_2) + (v_1, u_4) + (u_3, u_4)$, and then it is easy to know $T_1 \in T_n^*$. From Proposition 3, we know $x_{u_4} = x_{u_2}$; hence, $x_{u_4} = x_{u_2}$. And for $x_{u_4} > x_{u_2}$, then by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^*$. Hence, $x_{u_4} = x_{u_2}$.

Therefore, in conclusion, case 1 implies a contradiction.

**Case 2.** $i \geq 5$.

In this case, from Lemma 8, we have that $\min_{1 \leq i \leq 5} x_{u_i} < \max_{1 \leq i \leq 5} x_{u_i}$. Let $s$ be a vertex in $C$ such that $x_s = \min_{1 \leq i \leq 5} x_{u_i}$. From Theorem 12, we can get that there exists a natural number $i_0$ which satisfies $1 \leq i_0 \leq s \leq 1$ such that $x_{u_i} = \max_{1 \leq i \leq s} x_{u_i}$. Assume that $k$ is the number of the vertices whose components are equal to $\max_{1 \leq i \leq s} x_{u_i}$ in $C$. From $\min_{1 \leq i \leq s} x_{u_i} < \max_{1 \leq i \leq s} x_{u_i}$, we have $k \geq 1$. Suppose that $r_1, r_2, \ldots, r_k$ are all the vertices whose components are equal to $\max_{1 \leq i \leq s} x_{u_i}$ in $C$, and $r_1, r_2, \ldots, r_k$ are clockwise arrangement in $C$. Then, by Lemma 6, we can suppose that the vertices which follow the clockwise direction in $C$ are $s, r_1, r_2, \ldots, r_k, \ldots, s$ in sequence.

First, we can prove that $k \geq 2$ holds.

Assume that $k \geq 2$ is not established, then $k = 1$. Then, we can suppose that the vertices which follow the clockwise direction in $C$ are $w_2, \ldots, v_2, v_1, r_1, w_1, w_2$ in
sequence, where \( v_2, v_1, r_1, w_1 \), and \( w_2 \) are five different vertices in \( C \), and let the circle \( C \) be shown as Figure 10. From the definitions of \( r_1, r_2, \ldots, r_k \) and from \( k = 1 \), we can know that, for any natural number \( n \) which satisfies \( 1 \leq i \leq 2 \), we all have that \( x_{v_1} < x_{r_1} \) and \( x_{w_1} < x_{r_1} \) hold.

From Lemma 9, we can get \( N_{T_1}(w_1) \backslash V(C) \neq \emptyset \). Then for \( \forall t \in N_{T_1}(w_1) \backslash V(C) \), we all have that \( x_{v_1} < x_{r_1} \) holds. Otherwise, there exists \( t_1 \in N_{T_1}(w_1) \backslash V(C) \) such that \( x_{t_1} \geq x_{v_1} \).

Let \( T_1 = T^* - (w_1, t_1) - (r_1, v_1) + (r_1, t_1) + (w_1, v_1) \), then it is easy to know \( T_1 \in T_n^2 \). From \( x_{t_1} \geq x_{r_1} \) and \( x_{w_1} < x_{r_1} \), by Lemma 3, we have that \( \rho(T_1) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \).

Besides, we also can prove \( x_{v_1} < x_{w_1} \). Otherwise, \( x_{v_1} \geq x_{w_1} \); let \( T_2 = T^* - (v_1, v_2) - (r_1, w_1) + (r_1, v_2) + (w_1, v_1) \), then it is easy to know \( T_2 \in T_n^2 \). From the above conclusion, we have \( x_{v_1} < x_{r_1} \). For \( x_{v_1} < x_{r_1} \), by Lemma 3, we have that \( \rho(T_2) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \).

Choose \( t_2 \in N_{T_1}(v_1) \backslash V(C) \); let \( T_3 = T^* - (v_1, v_2) - (t_2, w_1) + (t_2, v_2) + (w_1, v_1) \), then it is easy to know \( T_3 \in T_n^2 \). From the above conclusion, we have \( x_{v_1} < x_{r_1} \). For \( x_{v_1} < x_{r_1} \), by Lemma 3, we have that \( \rho(T_3) > \rho(T^*) \) holds. This implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \). Hence, the hypothesis is not established; therefore, \( k \geq 2 \) holds.

Second, we can prove that \( l - k \geq 2 \) holds.

Assume that \( l - k \geq 2 \) is not established, then \( l - k = 1 \); hence, we can suppose that the vertices which follow the clockwise direction in \( C \) are \( s_1, r_1, r_2, \ldots, r_k \) in sequence. From \( l \geq 5 \), we know that \( k \geq 4 \) holds; thus \( s_1, r_1, r_{k-1}, \) and \( r_k \) are four different vertices.

Let \( T_4 = T^* - (r_1, s) - (r_{k-1}, r_k) + (r_1, r_k) + (s, r_{k-1}) \); it is easy to know \( T_4 \in T_n^2 \). From the definitions of \( r_1, r_2, \ldots, r_k \) and \( s \), we know \( x_{s_1} < x_{r_1} \). Since \( x_{s_1} < x_{r_1} \), by Lemma 3, we have that \( \rho(T_4) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \). Therefore, \( l - k = 1 \) is not established, then we have \( l - k \geq 2 \).

Denote \( m = l - k \), from \( l - k \geq 2 \), and we have that \( m \geq 2 \) holds. Then, we can suppose that the vertices which follow the clockwise direction in \( C \) are \( v_{m+1}, \ldots, v_1, r_1, \ldots, r_k \) in sequence. From \( m \geq 2 \) and \( k \geq 2 \), we know that \( v_{m+1}, v_1, r_1, \) and \( r_k \) are four different vertices in \( C \), and the relationship of the vertices of \( C \) is shown in Figure 11.

For the relationship between \( x_{v_1} \) and \( x_{v_{m+1}} \), we must have that \( x_{v_1} = x_{v_{m+1}} \) holds. Otherwise, there must exist one of the two equations, \( x_{v_1} < x_{v_{m+1}} \) and \( x_{v_1} > x_{v_{m+1}} \) holds. Let \( T_5 = T^* - (r_1, v_1) - (r_1, v_{m+1}) + (v_1, r_1) \), then it is easy to know \( T_5 \in T_n^2 \). If \( x_{v_1} < x_{v_{m+1}} \), for \( x_{r_1} \geq x_{v_1} \), by Lemma 3, we have that \( \rho(T_5) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \).

If \( x_{v_1} \geq x_{v_{m+1}} \), for \( x_{r_1} \leq x_{v_1} \), by Lemma 3, we have that \( \rho(T_5) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \). Hence, \( x_{v_1} = x_{v_{m+1}} \). Then, we have that \( x_{v_1} \geq x_{r_1} \) holds.

By Lemma 9, we know \( d(v_{m+1}) \geq 3 \); hence, \( N_{T_1}(v_{m+1}) \backslash V(C) \neq \emptyset \). Choose \( u \in N_{T_1}(v_{m+1}) \backslash V(C) \); then from Theorem 11, we get \( x_{u} < x_{r_1} \). Let \( T_6 = T^* - (r_1, v_1) - (u, v_{m+1}) + (v_{m+1}, u) \); it is easy to know \( T_6 \in T_n^2 \). From \( x_{v_1} \geq x_{r_1} \) and \( x_{r_1} < x_{v_1} \), by Lemma 3, we know that \( \rho(T_6) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^2 \).

Hence, in conclusion, case 2 implies a contradiction.

By consideration of the discussion of case 1 and case 2, we know that when \( l = 4 \) or \( l \geq 5 \), a contradiction is implied. Hence, \( l \geq 4 \) is not established; therefore, \( l = 3 \) and \( |V(C)| = 3 \). Then, we have that Theorem 16 holds.

Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^3 \), then the leaf nodes of \( T^* \) have the properties stated in the following theorem.

Theorem 17. Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T_n^3 \), and let \( r \) be the vertex that corresponds to a maximum component in the component of the Perron vector of \( T^* \). \( T^* \) is the rooted unicyclic graph with root node \( r \), let \( C \) be the only circle in \( T^* \), and \( V(C) = \{r, g_1, g_2\} \). Let \( d(u, v) \) be the shortest distance between vertex \( u \) and vertex \( v \) in \( T^* \), denote that \( W_1 = ||i|| \) is the leaf node of \( T^* \), and the shortest path from \( i \) to \( r \) neither pass \( g_1 \) nor pass \( g_2 \), \( W_2 = ||i|| \) is the leaf node of \( T^* \), and the shortest path from \( i \) to \( r \) either pass \( g_1 \) or pass \( g_2 \), then the following propositions are established:

1. If \( W_2 = \emptyset \), then \( \max_{i \in W} d(i, r) = 1 \).

2. If \( d(g_1) = 2 \), then for the arbitrary leaf node \( i \) in \( T^* \), we all have \( |1 - d(i, r)| \leq 1 \).

3. If \( W_2 \neq \emptyset \), then for the arbitrary leaves \( i, j \) in \( T^* \), we all have \( |d(i, j) - d(j, r)| \leq 1 \).
If $W_2 \neq \emptyset$, then $\min_{u \in W_2} d(i, r) \geq \max_{u \in W_2} d(j, r)$.

If $W_2 \neq \emptyset$, and there exists a vertex with degree 2 in $V(C)$, then $T^*$ is the rooted unicyclic graph with 3 levels, and for all $j \in W_1$, we have $d(j, r) = 1$.

Proof. Assume that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^*$, and suppose that $r$ is the vertex that corresponds to a maximum component in the component of the Perron vector of $T^*$, and $T^*$ is a rooted unicyclic graph with root node $r$. Suppose that $C$ is the only circle in $T^*$, and $V(C) = \{r, g_1, g_2\}$, let $x = (x_1, x_2, \ldots, x_n)^T$ be the Perron vector of $T^*$.

1. Assume that $\max_{u \in W_2} d(i, r) = 1$ is not established, then there exists a vertex $i \in W_1$ such that $d(i, r) \geq 2$. Suppose that the shortest path from $i$ to $r$ is $u_1u_2 \cdots u_r$, where $u_k = i,k \geq 2$. By Lemma 1, it is easy to prove that $x_{g_i} < x_{u_i}$ holds. And from Lemma 10, we get $x_{g_i} < x_{u_i}$. Let $T_1 = T^* - (g_1, g_2) - (u_1, u_2) + (u_1, g_2) + (g_1, u_2)$, it is easy to know $T_1 \in T_{n}^3$. From $x_{g_i} < x_{u_i}$ and $x_{u_i} > x_{u_1}$, by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T_n^*$. Hence, $\max_{u \in W_2} d(i, r) = 1$.

Therefore, (1) of Theorem 17 holds.

2. Assume that $d(g_i) = 2$, and there exists a leaf node $i$ in $T^*$ such that $|1 - d(i, r)| > 1$. Without loss of generality, we assume that the shortest path from $r$ to $i$ is $r^1v_1 \cdots v_k$, where $v_k = i$. From $|1 - d(i, r)| > 1$, we know $d(i, r) \geq 3$, then we have $k \geq 3$. Let $T_1 = T^* - (v_{k-1}, v_k) - (r, g_1) + (v_{k-1}, r) + (g_1, v_k)$, it is easy to know $T_1 \in T_{n}^*$. Since $x_{g_1} < x_{v_{k-1}}$, and from Lemma 10, we know that $x_{g_1} < x_{v_{k-1}}$. By Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T_n^*$; hence, $x_{g_1} < x_{v_{k-1}}$.

Let $T_2 = T^* - (v_{k-1}, v_k) - (r, g_1) + (v_{k-1}, r) + (g_1, v_k)$, it is easy to know $T_2 \in T_{n}^*$. Since $x_{g_1} < x_{v_{k-1}}$, and from Lemma 10, we know that $x_{g_1} < x_{v_{k-1}}$. By Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T_n^*$. Hence, when $d(g_1) = 2$, for any leaf node $i$ in $T^*$, we have that $|1 - d(i, r)| \leq 1$ holds. Similarly, when $d(g_i) = 2$, for any leaf node $i$ in $T^*$, we have that $|1 - d(i, r)| \leq 1$ holds.

Therefore, (2) of Theorem holds.

3. Assume that there exist two leaf nodes $i, j$ in $T^*$ such that $d(i, r) - d(j, r) = 1$. Suppose that $d(i, r) = k, d(j, r) = l$, then we have $|k - l| > 1$. Without loss of generality, we assume that $k - l > 1$, then we have that $k \geq l + 2$ and $l \geq 1$. Let $P_1$ be the shortest path from $i$ to $r$ and $P_2$ be the shortest path from $j$ to $r$. According to whether there is a public edge between $P_1$ and $P_2$, or not, we discuss the following two cases:

Case 1. There is no public edge between $P_1$ and $P_2$.

We denote the path $P_1$ by $r u_1v_{k-1} \cdots v_lw_1$, and the path $P_2$ by $ru_{l+1}u_{l+2} \cdots u_1$, where $v_1 = i$ and $u_1 = j$; $P_1$ and $P_2$ are shown in Figure 12. Besides, we denote $u_{r+1} = r$; by the definition of $r$, we know $x_{u_{r+1}} \geq x_{v_i}$. For $u_1$ is the leaf node in $T^*$ and $v_1$ is the nonleaf node in $T^*$, then by Lemma 10, we have $x_{u_1} < x_{v_1}$. From $x_{u_1} < x_{v_1}, x_{u_{r+1}} \geq x_{v_1}$ and $k - 1 \geq 1 + 1$, we know that there exists a natural number $s$ that satisfies $1 \leq s \leq l$, which makes $x_{u_1} < x_{u_{r+1}}$ and $x_{v_1} \geq x_{u_{r+1}}$. Let $T_1 = T^* - (u_{r+1}, u_{r+1}) - (v_{r+1}, v_{r+2}) + (v_{r+1}, u_{r+1}) + (u_1, v_{r+1})$, then it is easy to know $T_1 \in T_{n}^*$. From $x_{u_1} < x_{u_{r+1}}$ and $x_{v_1} \geq x_{u_{r+1}}$, by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T_{n}^*$. Case 2. There is a public edge between $P_1$ and $P_2$.

From that $W_2 \neq \emptyset, \Delta \geq 3$, and there exists public edge between $P_1$ and $P_2$, we know that there must exist a leaf node $w$ neither equal to $i$ nor equal to $j$, which makes the shortest path from $w$ to $r$ have no public edge with $P_1, P_2$. Denote the shortest path from the leaf node $w$ to $r$ by $P_3$, and then the length of $P_3$ is $l + 1$. Otherwise, the difference in length between $P_3$ and at least one of $P_1$ and $P_2$ is greater than 1. From the discussion of case 1, we know that this will lead to a contradiction. Besides, there will be $k = 2 + 1$. Otherwise, $k > 2 + 1$, it will imply that the difference in length between $P_3$ and $P_1$ is more than 1, and $P_3$ has no public edge with $P_1$. From the discussion of case 1, we know that this will lead to a contradiction.

Suppose that $P_1, P_2$, and $P_3$ are shown in Figure 13, where $P_1$ is $u_1u_2u_3 \cdots u_{r+1} \cdots u_2$, $P_3$ is $v_{l+1}v_2 \cdots v_{r+1} \cdots r$, where $v_0 = i, v_1 = j$, and there exists $t \geq 2$ such that, for $\forall j + 1$, we all have $u_1 = v_j$. Let $P_2$ be $w_1w_2w_3 \cdots w_{r+1} \cdots r$, where $w_1$ is denoted by $w_1$ and denote $u_r = r$.

Now, we consider the paths $P_1$ and $P_3$.

For $u_1$ is the leaf node in $T^*$ and $u_1$ is the nonleaf node in $T^*$, then by Lemma 10, we get $x_{u_1} < x_{v_1}$. If there exists a natural number $s$ that satisfies $1 \leq s \leq t$, which makes that both $x_{u_1} < x_{v_1}$ and $x_{u_{r+1}} \geq x_{v_1}$ hold. Let $T_1 = T^* - (u_{r+1}, u_{r+1}) - (v_{r+1}, v_{r+2}) + (v_{r+1}, u_{r+1}) + (u_1, v_{r+1})$, then it is easy to know $T_1 \in T_{n}^*$. From $x_{u_1} < x_{u_{r+1}}$ and $x_{v_1} \geq x_{u_{r+1}}$, by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T_{n}^*$. Hence, for any natural number $s$ which satisfies $1 \leq s \leq t, x_{u_1} < x_{v_1}$ and $x_{u_{r+1}} \geq x_{v_1}$ cannot hold meanwhile. And for $x_{u_1} < x_{v_1}$, then we have that, for any natural number $s$ which satisfies $1 \leq s \leq t$, we all have $x_{u_1} < x_{v_1}$.

Now we consider the paths $P_2$ and $P_3$.

For $v_2$ is the leaf node in $T^*$ and $w_2$ is the nonleaf node in $T^*$, by Lemma 10, we get $x_{v_2} < x_{w_2}$. Since $x_{v_{r+1}} = x_{u_{r+1}} > x_{w_{r+1}}$, then there exists a natural
number $s$ that satisfies $2 \leq s \leq t$, which make that both $x_{v_i} < x_{w_i}$ and $x_{v_{i+1}} \geq x_{w_{i+1}}$ hold. Let $T_2 = T^* - (v_{i}, v_{i+1}) - (w_{i}, w_{i+1}) + (w_{i+1}, v_{i+2}) + (v_{i+2}, w_{i+3})$, then it is easy to know $T_2 \in T^\Delta_n$. From $x_{v_i} < x_{w_i}$ and $x_{v_{i+1}} \geq x_{w_{i+1}}$, by Lemma 3, we know that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^\Delta_n$.

From the discussion of case 1 and case 2, we know that the hypothesis is not established. Therefore, (3) of Theorem 17 holds.

(4) Assume that the proposition is not established, then there exist vertices $i \in W_2$ and $j \in W_1$ such that $d(i, r) < d(j, r)$. From $i \in W_2$, we know $d(i, r) \geq 2$. Without loss of generality, we assume that the shortest path from $r$ to $i$ is $r v_1 v_2 \cdots v_s$ and the shortest path from $r$ to $j$ is $r w_1 w_2 \cdots w_k$, where $i = v_s$ and $j = w_k$. Then, we have that $k > s$ and $s \geq 2$ hold. From $i \in W_2$, we know that the shortest path from $i$ to $r$ must pass one of $g_1$ and $g_2$. Without loss of generality, we assume that the shortest path from $i$ to $r$ pass $g_1$, then $v_1 = g_1$. By (3) of Theorem 17, we know $k = s + 1$.

Since $v_s$ is the leaf node in $T^*$ and $w_{k-1}$ is the nonleaf node in $T^*$, then by Lemma 10, we get $x_{w_{k-1}} > x_{v_s}$. Let $T_1 = T^* - (v_{s-1}, v_s) - (w_{k-1}, w_{k-2}) + (w_{k-1}, v_{s-1}) + (v_{s-1}, w_{k-2})$, it is easy to know $T_1 \in T^\Delta_n$. From $x_{w_{k-1}} > x_{v_s}$, if $x_{w_{k-2}} \leq x_{v_{s-1}}$, by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds. This implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^\Delta_n$, hence, $x_{w_{k-2}} > x_{v_{s-1}}$. By mathematical induction, we get $x_{w_{k-i}} > x_{v_{s-i+1}}$, then we have that $x_{w_i} > x_{v_i}$ holds.

We also can prove that $x_{w_i} > x_{g_j}$ holds. Otherwise, $x_{w_i} \leq x_{g_j}$. For $x_{w_i} > x_{v_i}$, let $T_3 = T^* - (w_1, w_2) - (v_1, v_2) + (w_1, g_2) + (v_1, w_2)$, it is easy to know $T_3 \in T^\Delta_n$. From $x_{w_i} < x_{v_i}$ and $x_{w_1} > x_{v_1}$, by Lemma 3, we have that $\rho(T_3) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^\Delta_n$.

Let $T_3 = T^* - (w_1, w_2) - (v_1, v_2) + (w_1, g_2) + (v_1, w_2)$, it is easy to know $T_3 \in T^\Delta_n$. From $x_{v_1} \geq x_{w_1}$ and $x_{w_1} > x_{g_2}$, by Lemma 3, we have that $\rho(T_3) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^\Delta_n$.

Hence, the hypothesis is not established; therefore, (4) of Theorem 17 holds.

(5) Assume that $T^*$ is not a rooted unicyclic graph with levels 3, and since $W_2 \neq \emptyset$, then $T^*$ is a rooted unicyclic graph with levels not less than 4. For there exists a vertex with degree 2 in $V(C)$, without loss of generality, we assume that $d(g_2) = 2$. From $W_2 \neq \emptyset$, the level of $T^*$ is not less than 4 and (4) of Theorem 17, and we know that there exists a vertex $i \in W_2$ such that $d(i, r) \geq 3$. Suppose that the shortest path from $i$ to $r$ is $v_1 v_2 \cdots v_r$, where $v_1 = i$. Then, from $d(i, r) \geq 3$, we know that $k \geq 3$ holds, and from $d(g_2) = 2$, we know that $v_k = g_1$ holds. Let $T_1 = T^* - (v_1, v_2) - (r, g_3) + (r, v_3) + (g_2, v_3)$, from $v_2 = g_1$ and $k \geq 3$, we know $T_1 \in T^\Delta_n$. And by Lemma 1, it is easy to prove $x_{v_1} > x_{v_2}$. For $x_{v_1} \leq x_{v_2}$, then by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^\Delta_n$, hence, the hypothesis is not established. Therefore, $T^*$ is a rooted unicyclic graph with levels 3.

Next, we prove that, for $v \in W_1$, we all have $d(j, r) = 1$. Otherwise, assume that there exists a vertex $j_0 \in W_1$ such that $d(j_0, r) \geq 2$. And for $T^*$ is a rooted unicyclic graph with levels 3, then we have that $d(j_0, r) = 2$ holds. Suppose that the shortest path from $j_0$ to $r$ is $w_1 w_2 r$, where $w_1 = j_0$, $w_2$ is neither equal to $g_1$ nor equal to $g_2$. From that there exists a vertex with degree 2 in $V(C)$, without loss of generality, assume that $d(g_2) = 2$. Then, from Lemma 1, it is easy to prove $x_{g_1} \leq x_{w_2}$ holds. By Lemma 10, we can get $x_{w_2} > x_{w_1}$. Let $T_2 = T^* - (g_1, g_2) - (w_1, w_2) + (g_1, w_1) + (g_2, w_2)$, then it is easy to know $T_2 \in T^\Delta_n$. From $x_{w_2} > x_{w_1}$ and $x_{g_2} > x_{w_1}$, by Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^\Delta_n$.

Hence, the hypothesis is not established. Therefore, for $v j \in W_1$, we all have that $d(j, r) = 1$ holds.

In conclusion, (5) of Theorem 17 holds.

For the relationship between the maximal-adjacency-spectrum unicyclic graphs in $T^\Delta_n$ and the almost full-degree unicyclic graphs, we have the following theorem. \( \square \)
Theorem 18. Suppose that $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T^*_n$, $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $T^*$, and $r$ is the vertex that corresponds to a maximum component in the component of the Perron vector of $T^*$. Let $T^*$ be the rooted unicyclic graph with root node $r$, then $T^*$ is an almost full-degree unicyclic graph with root node $r$.

Proof. Suppose that the only circle in $T^*$ is $C$. From Theorem 16, we get $|V(C)| = 3$. By Theorem 12, we know $r \notin V(C)$, then $V(C) = \{r, g_1, g_2\}$. Denote $W_1 = \{i \mid i \text{ is the leaf node of } T^*\}$, and the shortest path from $i$ to $r$ neither pass $g_1$ nor pass $g_2$, $W_2 = \{i \mid i \text{ is the leaf node of } T^*, \text{ and the shortest path from } i \text{ to } r \text{ either pass } g_1 \text{ or pass } g_2\}$.

Now according to $T^*$, we discuss the following three cases:

Case 1. There exist nonfull internal vertices in $T^*$ and exist nonfull internal vertices in $C$.

For case 1, according to whether there exist vertices with degree 2 in $C$ or not, we discuss the following two subcases:

Subcase 1. There exist nonfull internal vertices in $C$ and exist the vertices with degree 2 in $C$.

For subcase 1, according to the number of the vertices with degree 2 in $C$, we continue to discuss the following two subcases:

Subcase 1.1. There are at least two vertices with degree 2 in $C$.

In this case, it is easy to know $W_2 = \emptyset$; by (1) of Theorem 17, we know $\max_{W_1} d(i, r) = 1$; thus, $T^* \cong T^*_{n, 2}$, where $T^*_{n, 2}$ is shown in Figure 2. Hence, $T^*$ is an almost full-degree unicyclic graph with root node $r$.

Subcase 1.2. There is only one vertex with degree 2 in $C$.

In this case, it is easy to know $W_2 \neq \emptyset$. For there is only one vertex with degree 2 in $C$, then by (5) of Theorem 17, we know that $T^*$ is a rooted unicyclic graph with levels 3. And for $\forall j \in W_1$, all we have that $d(j, r) = 1$ holds; hence, it is easy to know that $T^*$ is an almost full-degree unicyclic graph with root node $r$.

Subcase 2. There exist nonfull internal vertices in $C$, and the degree of all the vertices in $C$ is not equal to 2.

In this case, it is easy to know that the degree of all the vertices in $C$ are more than 2. From that, there exist nonfull internal vertices in $C$, and from Theorem 14, we know that there is only one nonfull internal vertex in $C$. Without loss of generality, assume that $g_1$ is the nonfull internal vertex in $C$, then we have that $d(g_1) = \Delta$ and $3 \leq d(g) \leq \Delta$ holds. And by Theorem 13, we know that there is only one nonfull internal vertex in $T^*$. Then, it is easy to know that $W_1 \neq \emptyset, W_2 \neq \emptyset$ and $\min_{W_1} d(i, r, d(i, r)) \geq 2$ hold.

Suppose $\max_{i \in W} d(i, r) = m$, then $m = 1$. Assume that $m = 1$ is not established, then we have $m \geq 2$. Now choose a vertex $u_1$ which satisfies $d(u_1, r) = r$ and $u_1 \in W_1$ in $T^*$. Choose $u_2 \in N_{T^*} (u_1)$, then $x_{g_1} \leq x_{u_2}$.

Otherwise, $x_{g_1} > x_{u_2}$, let $T_1 = T^* - (u_1, u_2) + (g_2, u_1)$, from $m \geq 2$ and $g_2$ is the nonfull internal vertex in $T^*$, we know $T_1 \in T^*_3$. And by Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T^*_n$. Let $T_2 = T^* - (g_1, g_2) - (u_1, u_2) + (g_2, u_1) + (u_2, g_1)$, it is easy to show $T_2 \in T^*_3$. From $x_{g_1} \leq x_{u_2}$, and by Lemma 10, we get $x_{g_1} > x_{u_2}$; then by Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T^*_3$.

Hence, the hypothesis is not established, and then we have $m = 1$. From $\min_{W_1} d(i, r) \geq 2$, we get $\max_{W_1} d(i, r) \geq 2$. And for $\max_{W_1} d(i, r) = 1$, by (3) of Theorem 17, we have that $\max_{W_1} d(i, r) = 2$. Thus, $\max_{W_1} d(i, r) = 2$, and from Theorem 17, we know that there is only one nonfull internal vertex in $T^*$, we know that $T^*$ is an almost full-degree unicyclic graph with root node $r$.

By consideration of the discussion of subcase 1 and subcase 2 in case 1, we know that if there exist nonfull internal vertices in $T^*$, and there exist nonfull internal vertices in $C$, then $T^*$ is an almost full-degree unicyclic graph with root node $r$.

Case 2. There exist nonfull internal vertices in $T^*$, and there is no nonfull internal vertex in $C$.

Since there exist nonfull internal vertices in $T^*$, and there is no nonfull internal vertex in $T^*$, then there exist nonfull internal vertices out of the circle of $T^*$. By Theorem 13, we know that there only one nonfull internal vertex in $T^*$.

We denote $r$ by $u_0$, let $w$ be the only nonfull internal vertex in $T^*$. Denote that $d(r, w) = l$, obviously, $l \geq 1$.

Choose a path $P_1$ in which $u_0$ is the starting point and a leaf node of $T^*$ is the terminal point, and $P_1$ passes $w$. Suppose that $P_1 = u_0, u_1, \ldots, u_l, u_1, \ldots, u_k$, where $k > l$. From the definition of $P_1$, we know $u_k = w$, then we have that $u_k$ is the only nonfull internal vertex in $T^*$.

Assume that $T^*$ is not an almost full-degree unicyclic graph with root node $r$. If $k = l + 1$, then from that there is only one nonfull internal vertex in $T^*$, and from Theorem 17, we have that, in $T^*$, there exists a path $P_2$ in which $u_0$ is the starting point and a leaf node of $T^*$ is the terminal point. Besides, $P_1$ has no public edge with $P_2$, and the length of $P_2$ is $l + 2$. Suppose that $P_2$ is $u_0, v_1, \ldots, v_{l+1}, v_{l+2}$, where $v_{l+2}$ is the leaf node, then the relationship between $P_1$ and $P_2$ is shown in Figure 14. If $k = l + 2$, then from that, there is only one nonfull internal vertex in $T^*$ and from Theorem 17, we know that, in $T^*$, there exists a path $P_1$ in which $u_0$ is the starting point and a leaf node of $T^*$ is the terminal point. Besides, $P_1$ has no public edge with $P_1$, and from Theorem 17, we know that the length of $P_1$ is not less than $l + 1$. Hence, suppose that $P_2$ is $u_0, v_{l+1}, \ldots, v_{l+1}, \ldots$, and the relationship between $P_1$ and $P_2$ is shown in Figure 15. If $k \geq l + 3$, from that there is only one nonfull internal vertex in $T^*$, and from Theorem 17, we know that, in $T^*$, there exists a path $P_4$ in which $u_0$ is the
starting point and a leaf node of $T^*$ is the terminal point. Besides, $P_i$ has no public edge with $P_1$, and from Theorem 17, we know that the length of $P_i$ is not less than $l + 2$. Hence, suppose that $P_i$ is $u_0v_1 \cdots v_{l+2}$, and the relationship between $P_1$ and $P_i$ is shown in Figure 16.

Now according to the relationship between $k$ and $l$, we discuss the following two subcases: let $k = l + 1$ or $k \geq l + 3$ be the subcase 1, and let $k = l + 2$ be the subcase 2.

Subcase 1. If $x_{u_i} \geq x_{v_{i+1}}$, let $T_1 = T^* - (v_{l+2}, v_{l+1}) + (v_{l+2}, u_{l+1})$, then it is easy to know $T_1 \in T^*_n$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^*_n$.

If $x_{u_i} < x_{v_{i+1}}$ and for $x_{u_i} = x_{\tau_i} \geq x_{v_i}$, we know that there exists a natural number $k$ that satisfies $2 \leq k \leq l + 1$, which makes that $x_{u_{k-1}} < x_{v_i}$ and $x_{u_{k-1}} \geq x_{v_{i+1}}$ hold. Let $T_2 = T^* - (v_{k-1}, v_k) + (u_{k-1}, u_k) + (v_{k-1}, u_{k-2})$, and it is easy to know $T_2 \in T^*_n$. From $x_{u_{k-1}} < x_{v_i}$ and $x_{u_{k-1}} \geq x_{v_{i+1}}$, and by Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T^*_n$.

Hence, subcase 1 of case 2 implies a contradiction.

Subcase 2. In subcase 2, according to whether $v_{i+1}$ is the leaf node or not, we discuss the following two subcases:

Subcase 2.1. $v_{i+1}$ is the leaf node.

In this case, by Lemma 10, we have $x_{u_{i+1}} < x_{v_{i+1}}$.

If $x_{v_i} \geq x_{u_i}$, and for $x_{v_i} < x_{u_i}$, let $T_1 = T^* - (v_{i+1}, v_i) + (u_{i+1}, u_i)$, then it is easy to know $T_1 \in T^*_n$. By Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^*_n$; hence, $x_{v_i} < x_{u_i}$. Let $T_2 = T^* - (v_i, v_{i+1}) + (u_{i+1}, u_i)$, it is easy to know $T_2 \in T^*_n$, and by Lemma 1, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^*_n$.

Subcase 2.2. $v_{i+1}$ is not the leaf node.

In this case, if there exists a natural number $i$ which satisfies $1 \leq i \leq l + 1$ such that $x_{v_i} < x_{u_i}$, then let $T_3 = T^* - (v_{i+1}, v_i) + (u_{i+1}, u_i)$, it is easy to know $T_3 \in T^*_n$. By Lemma 1, we have that $\rho(T_3) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^*_n$.

Hence, for arbitrary vertex $v_i$ which satisfies $1 \leq i \leq l + 1$, we all have $x_{v_i} \geq x_{u_i}$. Specially, we have $x_{u_{l+1}} > x_{v_{l+1}}$.

From $x_{u_{l+1}} > x_{v_{l+1}}$ and $x_{v_{l+1}} > x_{u_i}$, we know that there exists a natural number $k$ that satisfies $2 \leq k \leq l + 1$, which makes both $x_{u_{k-1}} > x_{u_{l+1}}$ and $x_{v_{k-1}} \geq x_{u_{l+1}}$ hold. Let $T_4 = T^* - (v_{k-1}, v_k) + (u_{k-1}, u_k) + (v_{k-1}, u_{k-2}) + (u_{k-1}, v_{k-1})$, it is easy to know $T_4 \in T^*_n$. From $x_{u_{k-1}} > x_{u_{l+1}}$ and $x_{v_{k-1}} \geq x_{u_{l+1}}$, by Lemma 3, we have that $\rho(T_4) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ being a maximal-adjacency-spectrum unicyclic graph in $T^*_n$.

Hence, in subcase 2, no matter whether $v_{i+1}$ is leaf node or not, it will imply a contradiction.

By consideration of the subcase 1 and subcase 2 in case 2, we know that the hypothesis is not established.
we know that when there exists nonfull internal vertices in \( T^* \), and there exists no nonfull internal vertices in \( C \), \( T^* \) is an almost full-degree unicyclic graph with root node \( r \).

Case 3. There is no nonfull internal vertex in \( T^* \), then there are only full-degree vertices and leaf nodes in \( T^* \). From Theorem 17, we know that \( T^* \) is an almost full-degree unicyclic graph with root node \( r \).

In conclusion, for each of the cases, \( T^* \) is still an almost full-degree unicyclic graph with root node \( r \), then we have that Theorem 18 holds.

Assume that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T^* \), \( T^* \neq T^* \), and there is only one nonfull internal vertex in \( T^* \), then from the position of the nonfull internal vertex in \( T^* \), we have the following conclusion, as in the following theorem.

**Theorem 19.** Suppose that \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T^* \), \( x = (x_1, x_2, \ldots, x_9) \) is the Perron vector of \( T^* \), \( r \) is the vertex that corresponds to a maximum component in the component of the Perron vector of \( T^* \), and \( T^* \) is the rooted unicyclic graph with root node \( r \), \( T^* \) has only one nonfull internal vertex \( u \). Suppose that \( C \) is the only one circle in \( T^* \), and \( V(C) = \{r, g_1, g_2\} \), denote that \( W_1 = [i] \) is the leaf node of \( T^* \), and the shortest path from \( i \) to \( r \) neither pass \( g_1 \) nor pass \( g_2 \), \( W_2 = [i] \) is the leaf node of \( T^* \), and the shortest path from \( i \) to \( r \) either pass \( g_1 \) or pass \( g_2 \).

Assume that \( T^* \neq T^* \) that is \( W_2 \neq \emptyset \), then the following propositions are established:

1. If the distances from all leaves of \( T^* \) to \( r \) are all equal, then there exists a leaf node \( i \in W_1 \) which makes \( (i, u) \) is a pendant edge.

2. If there are two leaves \( i, j \) in \( T^* \) which make \( d(i, r) \neq d(j, r) \) and \( \max_{i \in W_1} d(i, r) = \min_{i \in W_1} d(i, r) \), then either there exists a leaf node \( j \in W_2 \) which makes \( (u, j) \) is a pendant edge or \( u \in V(C) \) and \( d(u) = 2 \).

3. If \( \max_{i \in W_1} d(i, r) \neq \min_{i \in W_1} d(i, r) \), then there exists a leaf node \( j \in W_1 \) which makes \( (u, j) \) is a pendant edge.

**Proof.** From Theorem 18, we know that \( T^* \) is an almost full-degree unicyclic graph with root node \( r \); suppose that \( T^* \) is a rooted unicyclic graph with levels \( k \), then \( u \) is in the \( k - 1 \) level.

1. From \( W_2 \neq \emptyset \), we know \( \max_{i \in W_1} d(i, r) \geq 2 \); thus, \( T^* \) is a rooted unicyclic graph with the levels not less than 3. First, we have that \( d(g_1) \geq 3 \) and \( d(g_2) \geq 3 \) holds. Otherwise, there is at least one of the two equations, \( d(g_1) = 2 \) and \( d(g_2) = 2 \), holds. From \( W_2 \neq \emptyset \), we know that there is at most one of the two equations which are \( d(g_1) = 2 \) and \( d(g_2) = 2 \) holds. Hence, there is only one of the two equations which are \( d(g_1) = 2 \) and \( d(g_2) = 2 \) holds. By (5) of Theorem 17, we get that, for \( \forall j \in W_1 \), we all have that \( d(j, r) = 1 \) holds; hence, \( \max_{i \in W_2} d(i, r) = 1 \). Then, we can get \( \max_{i \in W_2} d(i, r) > \max_{i \in W_1} d(i, r) \), and this implies a contradiction with the distances from all leaves of \( T^* \) to \( r \) are all equal; hence, \( d(g_1) \geq 3 \) and \( d(g_2) \geq 3 \).

Assume that (1) of Theorem 19 is not established, then there exists \( u_i \in W_2 \) such that \( (u_i, u) \) is a pendant edge of \( T^* \). Let \( u_1, u_2, \ldots, u_m \) be the shortest path from \( u_i \) to \( r \), where \( u_1 = u \), \( u_m = g_1 \), or \( u_m = g_2 \). Without loss of generality, we assume that \( u_m = g_1 \), from \( u_1 \in W_2 \), we know \( m \geq 2 \).

For the range of the value of \( m \), we must have that \( m \geq 3 \) holds. Otherwise, \( m = 2 \), since the distances from all the leaf nodes in \( T^* \) to \( r \) are equal, then for \( \forall j \in W_1 \), we all have that \( d(j, r) = 2 \). Choose \( j \in W_1 \); let \( v_1, v_2, r \) be the shortest path from \( j \) to \( r \), where \( v_1 = j \), \( v_2 \neq g_1 \) and \( v_2 \neq g_2 \). By Lemma 10, we have that \( x_{g_1} > x_{v_1} \) and \( x_{g_2} \neq x_{v_1} \). Otherwise, \( x_{g_1} > x_{v_2} \), let \( T_1 = T^* - (v_1, v_2) + (v_1, g_1) \), and it is easy to know \( T_1 \in T^* \). By Lemma 11, we have that \( \rho(T_1) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T^* \).

Let \( T_2 = T^* - (g_1, g_2) - (v_1, v_2) + (g_2, v_2) + (g_1, v_1) \), then it is easy to know \( T_2 \in T^* \). From \( x_{g_1} > x_{v_1} \), and \( x_{g_2} \neq x_{v_1} \), by Lemma 3, we have that \( \rho(T_3) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T^* \). Thus, the hypothesis does not hold; that is, \( m \geq 3 \) holds.

Since for any two leaf nodes \( i, j \) in \( T^* \), we all have \( d(i, r) = d(j, r) \) and \( d(i, r) = d(j, r) \). And since \( d(u, r) = m \), then \( u \in W_2 \), then for \( \forall j \in W_1 \), we all have that \( d(j, r) = m \) holds. Choose \( j \in W_1 \), then we have that \( d(j, r) = m \) holds. Without loss of generality, we assume that the shortest path from \( j \) to \( r \) is \( v_1, v_2, \ldots, v_m, r \), where \( v_1 = j \), \( v_2 \neq g_1 \) and \( v_m \neq g_2 \).

Since \( u_1 = u \) is the nonfull internal vertex, then we have \( x_{u_1} < x_{v_1} \). Otherwise, \( x_{u_1} \geq x_{v_1} \), let \( T_3 = T^* - (v_1, v_2) + (v_1, u_2) \), and it is easy to know \( T_3 \in T^* \). By Lemma 11, we have that \( \rho(T_3) > \rho(T^*) \) holds, and this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T^* \).

Hence, \( x_{u_1} < x_{v_1} \).

For \( m \geq 3 \), hence \( u_1 \) and \( v_1 \) have the meaning. For the relationship between \( x_{u_1} \) and \( x_{v_1} \), we have that \( x_{u_1} < x_{v_1} \) holds. Otherwise, \( x_{u_1} \geq x_{v_1} \), let \( T_4 = T^* - (u_1, u_2) + (v_1, v_2) + (v_1, u_2) \), and it is easy to know \( T_4 \in T^* \). Since \( x_{u_1} \geq x_{v_1} \), and \( x_{u_1} < x_{v_1} \), by Lemma 3, we have that \( \rho(T_4) > \rho(T^*) \) holds, this implies a contradiction with \( T^* \) is a maximal-adjacency-spectrum unicyclic graph in \( T^* \).

By mathematics induction, we can prove that, for any natural number \( i \) which satisfies \( 2 \leq i \leq m \), we all have that \( x_{u_i} < x_{v_i} \) holds.
From Lemma 10, we can get $x_{u_i} > x_{v_i}$. For the relationship between $x_{u_i}$ and $x_{v_i}$, we have $x_{u_i} > x_{v_i}$.

Otherwise, $x_{u_i} \leq x_{v_i}$, let $T_5 = T^* - (u_i, u_2) - (v_1, v_2) + (v_1, u_2) + (v_2, u_2)$, and it is easy to know $T_5 \in T_n^\alpha$. From $x_{u_i} > x_{v_i}$ and $x_{u_i} \leq x_{v_i}$, by Lemma 3, we have that $\rho(T_3) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$. By mathematics induction, we can prove that, for any natural number $i$ which satisfies $2 \leq i \leq m$, we all have that $x_{u_i} > x_{v_{i-1}}$ holds.

Hence, we have $x_{u_m} > x_{v_m} > x_{v_{m-1}}$.

For the relationship between $x_{g_2}$ and $x_{v_{m-1}}$, we have $x_{g_2} > x_{v_{m-1}}$. Otherwise, $x_{g_2} \leq x_{v_{m-1}}$. Let $T_6 = T^* - (u_m, g_2) - (v_{m-1}, v_m) + (g_2, v_m)$, and it is easy to know $T_6 \in T_n^\alpha$. From $x_{g_2} < x_{v_{m-1}}$ and $x_{g_2} \leq x_{v_{m-1}}$, by Lemma 3, we have that $\rho(T_6) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$.

Thus, we have that $x_{g_2} > x_{v_{m-1}}$ holds, let $T_7 = T^* - (u_m, g_2) - (v_{m-1}, v_m) + (g_2, v_m) + (v_{m-1}, u_m)$, and it is easy to know $T_7 \in T_n^\alpha$. By Lemma 7, we have that $\rho(T_7) > \rho(T^*)$ holds, this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$.

In conclusion, the hypothesis does not hold; hence, (1) of Theorem 19 holds.

Assume that $T^*$ is not a complete graph, then the nonfull internal vertex $u$ in $T^*$ should satisfy that there exists $v_i \in W_1$ such that $(v_i, u)$ is a pedent edge. For there exist two leaf nodes $i, j \in T^*$ such that $d_i(r) \neq d_j(r)$ and $\max_{v_i \in W_1} d(i, r) = \min_{v_i \in W_1} d(i, r)$. Hence by Theorem 17, we know that $\max_{v_i \in W_1} d(j, r) = \max_{v_i \in W_1} d(j, r) + 1$; thus, $u$ is in the third last level of $T^*$, and this implies a contradiction with $T^*$ is an almost full-degree unicyclic graph with root node $r$. Hence, the hypothesis does not hold, and then, (2) of Theorem 19 holds.

Since $W_2 \neq \emptyset$ and $\max_{W_2} d(i, r) \neq \min_{W_2} d(i, r)$, by Theorem 17, we get $\max_{W_2} d(i, r) = \min_{W_2} d(i, r) = \max_{W_2} d(i, r) + 1$. And it is easy to know $\min_{W_2} d(i, r) \geq 1$; hence, $\max_{W_2} d(i, r) \geq 2$. From (5) of Theorem 17, we get that $d(g_1) \geq 3$ and $d(g_2) \geq 3$ hold.

Assume that (3) of Theorem 19 does not hold, since $d(g_1) \geq 3$ and $d(g_2) \geq 3$, the nonfull internal vertex $u$ in $T^*$ should satisfy that there exists $j_1 \in W_1$ such that $(j_1, u)$ is a pedent edge of $T^*$. From $W_2 \neq \emptyset$, $d(g_1) \geq 3$, and $d(g_2) \geq 3$, we have that $d(j_1, r) \geq 2$ holds.

Now we will prove that $d(j_1, r) \geq 3$. Assume that $d(j_1, r) \geq 3$ does not hold, then we have $d(j_1, r) = 2$, by $\max_{W_2} d(i, r) = \min_{W_2} d(i, r) = \max_{W_2} d(i, r) = \min_{W_2} d(i, r) \geq 3$ and $d(g_1) \geq 3$ does not hold. We get $d(j_1, r) \geq 2$.

By Lemma 10, we can get $x_{u_i} > x_{v_i}$. For the relationship between $x_{u_i}$ and $x_{v_i}$, we have $x_{u_i} > x_{v_i}$. Otherwise, $x_{u_i} \leq x_{v_i}$. Let $T_5 = T^* - (u_i, u_2) - (v_1, v_2) + (v_1, u_2) + (v_2, u_2)$, and it is easy to know $T_5 \in T_n^\alpha$. From $x_{u_i} > x_{v_i}$ and $x_{u_i} \leq x_{v_i}$, by Lemma 3, we have that $\rho(T_5) > \rho(T^*)$ holds. This implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\alpha$. By mathematics induction, we can prove that, for any natural number $i$ which satisfies $2 \leq i \leq m + 1$, we all have that $x_{u_i} > x_{v_{i-1}}$ holds.
Hence, we have $x_{i_{x_{mn}}} > x_{i_{vm1}} > x_{i_{vn}}$. Besides, for the relationship between $x_{i_{g1}}$ and $x_{i_{vm1}}$, we have $x_{i_{g1}} < x_{i_{vm1}}$. Otherwise, $x_{i_{g1}} < x_{i_{vm1}}$. Let $T_6 = T^* - (g_1, g_2) - (v_{m_1}, v_{m_2}) + (g_1, v_{m_1}) + (g_2, v_{m_2})$, then it is easy to know $T_6 \in T_n^\Delta$. By $g_1 = t_{m_1}$ and $x_{i_{g1}} > x_{i_{vm1}}$, we can get $x_{i_{g1}} > x_{i_{vm1}}$. And for $x_{i_{g1}} < x_{i_{vm1}}$, by Lemma 3, we have that $\rho(T_6) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$. Let $T_7 = T^* - (g_2, v_{m_1}) - (v_{m_1}, v_{m_2}) + (g_2, v_{m_1}) + (u_{m_1}, v_{m_2})$, then it is easy to know $T_7 \in T_n^\Delta$. From $x_{i_{g2}} > x_{i_{vm1}}$ and $x_{i_{vm1}} > x_{i_{vm2}}$, we can get $x_{i_{g2}} > x_{i_{vm2}} > x_{i_{vm1}} > x_{i_{vn}}$. By Lemma 7, we have $\rho(T_7) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

In conclusion, the hypothesis does not hold, and hence, (3) of Theorem 19 holds.

Finally, we give the structure of the maximal-adjacency-spectrum unicyclic graphs in the set of unicyclic graphs given between the vertices and the maximum degree; in the following Theorem, we describe the structure of the maximal-adjacency-spectrum unicyclic graphs in $T_n^\Delta$.

**Theorem 20.** Suppose that $T^* \in T_n^\Delta$, and $T^*$ is a rooted unicyclic graph with root vertex which is the vertex that corresponds to a maximum component in the component of the Perron vector of $T^*$, then $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$ if and only if $T^* \equiv H_n^\Delta$.

**Proof.** Necessity. Suppose that $T^* \in T_n^\Delta$, $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, let $x = (x_1, x_2, \ldots, x_\ell)$ be the Perron vector of $T^*$, and $r$ be the vertex that corresponds to a maximum component of $x$. Suppose that $T^*$ is a rooted unicyclic graph with root node $r$; from Theorem 18, we have that $T^*$ is an almost full-degree unicyclic graph with root node $r$.

Denote the only circle in $T^*$ by $C$; from Theorem 16, we have $|V(C)| = 3$. Again by Theorem 12, we could suppose that $V(C) = \{r, g_1, g_2\}$. Denote $W_1 = [i|i]$ is the root node of $T^*$, and the shortest path from $i$ to $r$ neither pass $g_1$ nor pass $g_2$, $W_2 = [i|i]$ is the root node of $T^*$, and the shortest path from $i$ to $r$ either pass $g_1$ or pass $g_2$.

When the level of $T^*$ is 2, obviously, $T^* \equiv H_n^\Delta$.

When the level of $T^*$ is 3, if there is no nonfull internal vertex in $C$, then it is easy to know that $T^* \equiv H_n^\Delta$ holds. If there exists nonfull internal vertex in $C$, then according to the degree of the nonfull internal vertex in $C$, we discuss the following two cases:

**Case 1.** There is one nonfull internal vertex in $C$ with degree $2$.

In this case, we can prove $\max(d(g_1), d(g_2)) > 2$. Otherwise, $\max(d(g_1), d(g_2)) = 2$; that is, we have that $d(g_1) = d(g_2) = 2$ holds, and thus, $W_2 = \emptyset$. From (1) of Theorem 17, we know $T^* \equiv T_n^\Delta$, then $T^*$ is a rooted unicyclic graph with levels 2, and this implies a contradiction with the level of $T^*$ is 3. Without loss of generality, we assume that $\max(d(g_1), d(g_2)) = d(g_1)$; hence, $d(g_1) > 2$. And for there is one nonfull internal vertex with degree 2 in $C$, hence $d(g_2) = 2$, by (5) of Theorem 17, we get that, for $\forall i \in W_1$, we all have that $d(i, r) = 1$ holds. Therefore, $T^* \equiv H_n^\Delta$.

**Case 2.** The degree of all the nonfull internal vertices in $C$ is not less than 3.

In this case, from Theorem 14, we can get that there is only one nonfull internal vertex in $C$. Without loss of generality, we assume that $g_2$ is the nonfull internal vertex. For the degree of all the nonfull internal vertices in $C$ are not less than 3, the level of $T^*$ is 3, and $V(C) = \{g_1, g_2\}$; we have $\max_{j\in W_1} d(j, r) = min_{j\in W_1} d(j, r) = 2$. Then, by (4) of Theorem 17, we get $\max_{j\in W_1} d(j, r) < 2$.

We can prove $\max_{j\in W_1} d(j, r) = 1$. Otherwise, there exists $i \in W_1$ such that $d(i, r) = 2$. Suppose that the shortest path from $i$ to $r$ is $r_{u_1}u_{t_1}$, where $u_1 = i$ and $u_2$ is neither $g_1$ nor $g_2$. According to the relationship between $g_1$ and $x_{i_{g1}}$, we have $x_{i_{g1}} < x_{u_1}$. Otherwise, $x_{i_{g1}} > x_{u_1}$, let $T_1 = T^* - (u_1, u_2) + (u_1, g_2)$, and it is easy to know $T_1 \in T_n^\Delta$. By Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$. Let $T_2 = T^* - (u_1, u_2) - (g_1, g_2) + (g_1, u_2) + (u_1, g_2)$, then it is easy to know $T_2 \in T_n^\Delta$. Again by Lemma 10, we get $x_{i_{g1}} > x_{u_2}$. And we have proved $x_{i_{g1}} < x_{u_2}$; hence, by Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds. This implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$.

In conclusion, when the level of $T^*$ is 3, we have that $T^* \equiv H_n^\Delta$ holds.

Now we discuss the case in which the level of $T^*$ is not less than 4.

Suppose that $\max_{i\in W_1\cup W_2} d(i, r) = k$, from the level of $T^*$ is not less than 4, we know $k \geq 3$.

Denote $Q_1 = \{i \in V(T^*)|d(i, r) = k - 1\}$, and the shortest path from $i$ to $r$ pass neither $g_1$ nor $g_2$.

Denote $Q_2 = \{i \in V(T^*)|d(i, r) = k - 1\}$, and the shortest path from $i$ to $r$ pass either $g_1$ or $g_2$.

From Theorem 18, we get that $T^*$ is an almost full-degree unicyclic graph, then if there exists nonfull internal vertex in $T^*$, we have that the nonfull internal vertex in the second last level of $T^*$. And since the level of $T^*$ is not less than 4, if there exists nonfull internal vertex in $T^*$, then the nonfull internal vertex must belong to the set of $V(T^*)\setminus V(C)$. Again from Theorem 13, we get that there is only one nonfull internal vertex in $T^*$. Thus, when the level of $T^*$ is not less than 4, there is at most one nonfull internal vertex in $T^*$.

When the level of $T^*$ is not less than 4, we discuss the following three cases according to the structure of $T^*$.
Case 1. There is no nonfull internal vertex in $T^*$. At this time, we can discuss the following three subcases:

Subcase 1. When for arbitrary leaf nodes $i, j$ in $T^*$, we all have $d(i, r) = d(j, r)$.

At this time, it is easy to know that $T^* \cong H_n^\Delta$ holds.

Subcase 2. When there exist two leaf nodes $i, j$ in $T^*$ such that $d(i, r) \neq d(j, r)$ and $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r)$.

At this time, from Theorem 17, we get $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r) = \max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r) - 1 = k - 1$. And for $\forall q_1 \in Q_1$, we all have that $d(q_1) = \Delta$ holds.

Subcase 3. When $\max_{\mathcal{W}_1}d(i, r) \neq \min_{\mathcal{W}_1}d(i, r)$.

At this time, from Theorems 17 and 19, we know that the following two conclusions hold: $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r) = 1$ and $\forall q_2 \in Q_2$, we all have that $d(q_2) = \Delta$ holds.

Case 2. There is only one nonfull internal vertex $u$ in $T^*$, and one of the brothers of $u$ is leaf node.

Now, it is easy to know that there exist two leaf node nodes $i, j$ in $T^*$ such that $d(i, r) \neq d(j, r)$; then according to case (2), we discuss the following two subcases:

Subcase 1. When there exist two leaf nodes $i, j$ in $T^*$, which make $d(i, r) = d(j, r)$ and $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r)$.

At this time, from Theorems 17 and 19, we know that the following three conclusions hold: $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r) = 1$; $\forall q_1 \in Q_1$, we have that $d(q_1) = \Delta$ holds; $\forall q_2 \in Q_2$, we all have that $d(q_2) = \Delta$ holds.

Case 3. There is only one nonfull internal vertex $u$ in $T^*$, and all the brothers of $u$ are full-degree vertices.

According to case (3), we could discuss the following three subcases:

Subcase 1. When arbitrary leaf nodes $i, j$ in $T^*$ all have $d(i, r) = d(j, r)$.

At this time, from Theorem 19, we get that the nonfull internal vertex $u \in Q_2$. Since there exist two leaf node nodes $i, j$ such that $d(i, r) = d(j, r)$ and $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r)$ in $T^*$, by Theorem 17, we get $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r) = k - 1$.

Subcase 3. When $\max_{\mathcal{W}_1}d(i, r) \neq \min_{\mathcal{W}_1}d(i, r)$.

At this time, from Theorem 19, we get $u \in Q_2$. Since $\max_{\mathcal{W}_1}d(i, r) \neq \min_{\mathcal{W}_1}d(i, r)$, by (3) and (4) of Theorem 17, we can get $\max_{\mathcal{W}_1}d(i, r) = \min_{\mathcal{W}_1}d(i, r) = \max_{\mathcal{W}_1}d(i, r) + 1$. And for there is only one nonfull internal vertex $u$ in $T^*$, and $u \in Q_2$; hence, for $\forall q_2 \in Q_2$, we all have that $d(q_2) = \Delta$.

In the following, we call the subcases (3.2) and (3.3) “case 3" and the subcases (1.2), (1.3), (2.1), and (2.2) “case 4”.

Since $\max_{\mathcal{W}_1}d(i, r) = k (k \geq 3)$, we have that $T^*$ is a rooted unicyclic graph with levels $k + 1$.

Now according to the notation of the vertices in $T^*$, we make the following instructions: $\circ$ except $r, g_1, g_2$, if $w_1 \in V(T^*)$, then let $w_1$ express one of the vertices in the bottom layer of the first $i$ of $T^*$; $\circ$ If $w_1 \in V(T^*)$, we denote $w_1 (j > i)$ the ancestor of $w_1$, which is in the bottom layer of the first $i$ of $T^*$, (note: $w_1$ can equal to any one of the vertex $r$, $g_1$, $g_2$, and $g_1$ does not express that $g_1$ is in the first last level of $T^*$ and $g_2$ does not express that $g_2$ is in the second last level of $T^*$). The above notations in $\circ$ and $\circ$ are still established when $w$ is changed for any other vertex, which is not $g$.

Assume that $T^* \neq H_n^\Delta$, then the structure of $T^*$ must be as the following case 3 or case 4 shown.

Case 3. From the discussion of subcases 3.2 and 3.3, we know that there must exist a leaf node $s_2$ and an nonfull internal vertex $u$ in $T^*$ (it is easy to know that $u$ is in the second last level of $T^*$, denote $r_1 = u$), which make $u, s_2$ satisfy the following properties: $\circ$ $s_2$ at least has one full-degree brother. $\circ$ The common direct ancestor of $s_1$ and $u$ of the nearest generation is in the bottom layer of the first $l$ of $T^*$, and $l \geq 4$. We choose $v_2$ a full-degree brother of $s_2$, denote the common direct ancestor of $s_2$ and $u$ of the nearest generation is $r_1 (l \geq 4)$, then the relationship of the vertices in case 1 is shown in Figure 17, where in Figure 17, $u_2$ is a brother of $u$ and $d(u_2) = \Delta$.

If $x_{r_2} \geq x_{v_2}$, then let $T_1 = T^* - (v_1, v_2) + (v_1, r_2)$, it is easy to know $T_1 \cong T_n^\Delta$. And by Lemma 1, we can get $\rho(T_1) > \rho(T^*)$, and this implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, hence, $x_{r_2} > x_{v_2}$. And from Theorem 20, we know $x_{r_2} > x_{s_2}$.

Let $T_2 = T^* - (s_2, s_3) - (r_2, r_3) + (r_2, s_3) + (s_2, r_3)$, and it is easy to know that $T_2 \cong T_n^\Delta$. If $x_{r_2} \leq x_{s_2}$, from $x_{r_2} > x_{s_2}$, and by Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds. This implies a contradiction with $T^*$ is a maximal-adjacency-spectrum unicyclic graph in $T_n^\Delta$, hence, $x_{r_2} > x_{s_2}$. Let $T_3 = T^* - (v_2, s_3) - (r_2, r_3) + (r_2, s_3) + (s_2, r_3)$.
(v_2, r_3), then it is easy to know that T_3 \in T_n^\Delta. From x_{r_2} < x_{s_2} and x_{r_3} \geq x_{s_3}, by Lemma 3, we have that 
\rho(T_{r_2}) > \rho(T^*) holds. This implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta. Hence, the hypothesis is not established; therefore, 
T^* \equiv H_n^\Delta.

Case 4. For T^* is an almost full-degree unicyclic graph with root node r, T^* \not\equiv H_n^\Delta, and from the discussion of subcase 1.2, subcase 1.3, subcase 2.1, and subcase 2.2, we know that there must exist two leaf nodes r_2, s_2 in the second level of T^*, which satisfy the following properties.

There is a cousin or brother u_t of the nonleaf vertex which is of the nearest generation of r_2, there also exists a cousin or brother v_2 of the nonleaf vertex which is of nearest generation of s_2. This makes that r_t (where t \geq 3) is the common direct ancestor of r_2 and u_2 of the nearest generation, s_m (where m \geq 3) is the common direct ancestor of s_2 and v_2 of the nearest generation, w is the common direct ancestor of r_2, u_2, s_2, and v_2 of the nearest generation, and u_2 and v_2 satisfy that u_2 \neq v_2, r_t \neq u_t, s_m \neq w and r_t \neq s_m.

Without loss of generality, we assume that t \geq m. Then, the relationship of the vertices in case 2 is shown as Figure 18. From the method of marking the index of the vertices in T^*, we know r_t = u_t, s_m = v_m, and s_t = v_t.

First, by Lemma 10, it is easy to know max{x_{u_t}, x_{s_m}} < min{x_{u_t}, x_{s_m}}.

If x_{u_t} < x_{s_m}, then x_{u_t} \geq x_{v_m}. Since x_{u_t} < x_{v_m}, there is a natural number k that satisfies 2 \leq k \leq t - 1, which makes x_{u_{k+1}} < x_{s_{k+1}} and x_{u_{k+1}} \geq x_{s_{k+1}}. Let T_k = T^* - (r_{k+1}, r_k) - (r_{k+1}, v_k) + (v_{k+1}, r_k), then it is easy to know T_k \in T_n^\Delta. From x_{r_{k+1}} < x_{v_{k+1}} and x_{r_{k+1}} \geq x_{v_{k+1}}, by Lemma 3, we have that \rho(T_k) > \rho(T^*) holds, and this implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta.

If x_{u_t} < x_{s_m}, since x_{u_t} > x_{s_t}, there exists a natural number k that satisfies 2 \leq k \leq t - 1, which makes x_{u_{k+1}} > x_{s_{k+1}} and x_{u_{k+1}} \leq x_{s_{k+1}}. Let T_k = T^* - (u_{k+1}, u_k) - (s_{k+1}, s_k) + (u_{k+1}, s_k) + (s_{k+1}, u_k), then it is easy to know T_k \in T_n^\Delta. From x_{u_{k+1}} > x_{s_{k+1}} and x_{u_{k+1}} \leq x_{s_{k+1}}, by Lemma 3, we have that \rho(T_k) > \rho(T^*) holds, and this implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta.

Hence, the hypothesis is not established; therefore, 
T^* \equiv H_n^\Delta.

In conclusion, if T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta, and the level of T^* is not less than 4, we have that T^* \equiv H_n^\Delta holds.

By considering the discussion of all the cases according to the level of T^*, we know that if T^* \not\in T_n^\Delta, T^* is a unicyclic graph in which the vertex corresponding to a maximum component in the component of the Perron vector of T^* is the root node, and T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta, then T^* \equiv H_n^\Delta.

 Sufficiency, suppose that T^* \notin T_n^\Delta, T^* is a rooted unicyclic graph in which the vertex corresponding to a maximum component in the component of the Perron vector of T^* is the root node, and T^* \equiv H_n^\Delta. It is easy to know \rho(T^*) \neq \rho(H_n^\Delta), there must exist maximal-adjacency-spectrum unicyclic graph in T_n^\Delta. Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta, and let T^* be a rooted unicyclic graph in which the vertex corresponding to a maximum component in the component of the Perron vector of T^* is the root node. Then by the necessity of Theorem 20, we know T^* \equiv H_n^\Delta. And for T^* \not\equiv H_n^\Delta, then T^* \equiv H_n^\Delta; thus, T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^\Delta.

From Theorem 20, we know that if we regard the isomorphic graphs as one graph, then there is only one maximal-adjacency-spectrum unicyclic graph in T_n^\Delta and the maximal-adjacency-spectrum unicyclic graphs in T_n^\Delta is H_n^\Delta.

\[ \square \]

4. A New Upper Bound on the Adjacency Spectral Radius of the Unicyclic Graphs

In the following, on the basis of Theorem 20, we give a new upper bound on the adjacency spectral radius of the unicyclic graphs.

4.1. A New Upper Bound on the Adjacency Spectral Radius of the Unicyclic Graphs

About the upper bound on the adjacency spectral radius of the unicyclic graphs, Hu [3] has given that if T \in T_n^\Delta, then one upper bound of \rho(T) is 2\sqrt{\Delta - 1}.

Suppose that T \in T_n^\Delta, where T = (V(T), E(T)). Let C be the only circle in T, and suppose that V(C) = \{v_1, v_2, \ldots, v_r\}. Then, T - E(C) is a forest composed of B_1, B_2, \ldots, B_r, where B_1, B_2, \ldots, B_r are the rooted trees with the roots v_1, v_2, \ldots, v_r, respectively.

Denote

\[ K(T) = \max_{v \in V(T)} \{|d(v, u) - u \in V(B_i)| + 1 \} \]

Rojo [15] has given another upper bound on the adjacency spectral radius of the unicyclic graphs through the following theorem.

**Theorem 21** (see [15]). Assume that T \in T_n^\Delta, if \Delta = 3 and K(T) \geq 4, or \Delta = 4, \rho(T) < 2\sqrt{\Delta - 1} \cos(\pi / (2K(T) + 1)).
In order to give a new upper bound on the adjacency spectral radius of the unicyclic graphs, we first introduce some definitions and lemmas.

**Definition 8.** For the given natural number $n$ and $\Delta$, which satisfy $n > \Delta \geq 3$. We suppose that $F_1$ is a unicyclic graph with the maximum degree $\Delta$, and let $C_1$ be the only circle in $F_1$, $r$ be the vertex which corresponds to a maximum component in the components of the Perron vector of $F_1$, $F_1$ be the rooted unicyclic graph with root node $r$, and $F_1$ satisfies the following properties:

1. $F_1$ is an almost completely full-degree unicyclic graph with the maximum degree $\Delta$.
2. $\rho(F_1) \geq \rho(H_n^\Delta)$.
3. There is no nonfull internal vertex in $F_1$.
4. Let the set of the vertices of $C_1$ which is the only circle in $F_1$ be $V(C_1) = \{r, g_1, g_2\}$, denote $W_1(F_1) = \{i\}$ is the leaf node of $F_1$, and the shortest path from $i$ to $r$ neither pass $g_1$ nor pass $g_2$, $W_2(F_1) = \{i\}$ is the leaf node of $F_1$, and the shortest path from $i$ to $r$ either pass $g_1$ or pass $g_2$, then we have that $\min_{e \in W_1(F_1)} d(i, r) + 1 = \max_{e \in W_1(F_1)} d(i, r) + 1 = \min_{e \in W_2(F_1)} d(i, r) = \max_{e \in W_2(F_1)} d(i, r)$ hold.

Then, we call $F_1$ is a completely Bethe unicyclic graph with the maximum degree $\Delta$, the length of the circle is 3, and the adjacency spectral radius is not less than $\rho(H_n^\Delta)$.

**Definition 9.** According to the given natural number $n$ and $\Delta$, which satisfy $n > \Delta \geq 3$. Let $F$ be a completely Bethe unicyclic graph with the maximum degree $\Delta$, the length of the circle is 3, and the adjacency spectral radius is not less than $\rho(H_n^\Delta)$. If for any completely Bethe unicyclic graph $F_1$ with the maximum degree $\Delta$, the length of the circle is 3 and the adjacency spectral radius is not less than $\rho(H_n^\Delta)$, we all have that $\rho(F_1) \geq \rho(F)$ holds, then we call $F$ is the minimum completely Bethe unicyclic graph with the maximum degree $\Delta$, the length of the circle is 3, and the adjacency spectral radius is not less than $\rho(H_n^\Delta)$. We denote the minimum completely Bethe unicyclic graph with the maximum degree $\Delta$, the length of the circle is 3, and the adjacency spectral radius is not less than $\rho(H_n^\Delta)$ by $F_{n, \Delta}^\ast$.

Through the direct calculation, we have $K(F_{n, \Delta}^\ast) = \lceil \log_{\Delta - 1} (n/3) \rceil + 1$, where $[x]$ denotes the smallest positive integral which is not less than $x$.

For convenience, in the following proof process, now we give another notation of $F_{n, \Delta}^\ast$.

Denote $a(n, \Delta) = K(F_{n, \Delta}^\ast), m(n, \Delta) = |V(F_{n, \Delta}^\ast)|$, it is easy to know $a(n, \Delta) = \lceil \log_{\Delta - 1} (n/3) \rceil + 1$, and the orderly array $(a(n, \Delta), m(n, \Delta))$ is only determined by $(n, \Delta)$. Besides, it is easy to know that if there exist the natural number $n$ and $\Delta$ that satisfy $n > \Delta \geq 3$, which make the natural number $a$ and $m$ satisfy $a = K(F_{n, \Delta}^\ast)$ and $m = |V(F_{n, \Delta}^\ast)|$. Then, $\Delta$ is only determined by the orderly array $(a, m)$; that is, there exist the natural number $n$ and $\Delta$ that satisfy $n > \Delta \geq 3$, which make that the natural number $a$ and $m$ satisfy $a = K(F_{n, \Delta}^\ast), m = |V(F_{n, \Delta}^\ast)|$. Thus, the orderly array $(a, m)$ can only determine the structural of $F_{n, \Delta}^\ast$, which satisfies $a = K(F_{n, \Delta}^\ast) \ast m = |V(F_{n, \Delta}^\ast)|$. Hence, we can denote $F_{n, \Delta}^\ast$ by $F_{m(n, \Delta)}^\ast$. It is easy to know that if denote $a = \lceil \log_{\Delta - 1} (n/3) \rceil + 1$, then we have that $F_{n, \Delta}^\ast = F_{m(n, \Delta)}^\ast$.

**Lemma 11.** (see [16]). Suppose that $T \in T_n^{\Delta},$ where $\Delta \geq 3,$ if denote $a = \lceil \log_{\Delta - 1} (n/3) \rceil + 1$, then we have that $\rho(B_m(n, \Delta)) = \rho(A_n)$ holds.

**Lemma 12.** Suppose that $T \in T_n^{\Delta},$ where $\Delta \geq 3,$ if denote $a = \lceil \log_{\Delta - 1} (n/3) \rceil + 1$, then when $\Delta = 3$ and $a \geq 4$, or when $\Delta \geq 4$, we have that $\rho(B_m(n, \Delta)) < 2\sqrt{\Delta - 1} \cos(\pi/(2a + 1))$ holds.

**Proof.** By the definition of $B_m(n, \Delta)$ and Theorem 21, it is easy to prove that Lemma 12 holds.

Now we give a new upper bound on the adjacency spectral radius of the unicyclic graphs, that is, the following theorem.

**Theorem 22.** Suppose that $T \in T_n^{\Delta},$ then the following holds:

1. When $\Delta = 3$ and $n \leq 6$, we have that $\rho(T) \leq 1 + \sqrt{2}$ holds, and the necessary and sufficient condition for the equal sign establishes is $T \equiv B_6^\ast$, that is $T \equiv H_6^\ast$.
2. When $\Delta = 3$ and $7 < n \leq 12$, we have that $\rho(T) \leq \rho_1$ holds, where $\rho_1$ is the maximum real root of the
Proof. (1) When $\Delta = 3$ and $n \leq 6$, it is easy to know $F_{n,3}^* = B_{6}^3$; by the definition of $B_{6}^3$ and Theorem 20, it is easy to have that $\rho(T) \leq \rho(B_{6}^3)$ holds. From Theorem 20, we know that the equal sign establishes if and only if $T \equiv H_{12}^3$. If we denote $A_2 = \begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix}$, then from Lemma 11, we know that $\rho(B_{6}^3) = \rho(A_2)$ holds. Hence, we have $\rho(T) \leq \rho(A_2)$, through direct calculation, we get $\rho(A_2) = 1 + \sqrt{2}$; thus, we have that $\rho(T) \leq 1 + \sqrt{2}$ holds.

From the above proof process, we know that the necessary and sufficient condition for the equal sign in the inequality $\rho(T) \leq 1 + \sqrt{2}$ establish is $T \equiv H_{12}^3$, that is, $T \equiv H_{12}^3$.

(2) When $\Delta = 3$ and $7 < n \leq 12$, it is easy to know $F_{n,3}^* = B_{12}^3$; by the definition of $B_{12}^3$ and by Theorem 20, it is easy to have that $\rho(T) \leq \rho(B_{12}^3)$ holds, and from Theorem 20, we know that the equal sign establishes if and only if $T \equiv B_{12}^3$.

If denoted $A_3 = \begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$, then from Lemma 11, we know that $\rho(B_{12}^3) = \rho(A_3)$ holds. Hence, we have $\rho(T) \leq \rho(A_3)$, through the direct calculation, we get that $\rho(A_3)$ is the maximum real root of the equation $\lambda^3 - 2\lambda^2 - 3\lambda + 2 = 0$. Denote the maximum real root of the equation $\lambda^3 - 2\lambda^2 - 3\lambda + 2 = 0$ by $\rho_1$; thus, we have that $\rho(T) \leq \rho_1$ holds.

From the above proof process, we know that the necessary and sufficient condition for the equal sign in the inequality $\rho(T) \leq \rho_1$ established is $T \equiv B_{12}^3$, that is, $T \equiv H_{12}^3$.

(3) When $\Delta = 3$ and $n \geq 13$, or when $\Delta \geq 4$, by the definition of $\rho_1$, we have $\rho(T) \leq \rho_1$. By the definition of $B_{m(n,3)}^*$ and Theorem 20, we have that $\rho(T) \leq \rho(B_{m(n,3)}^*)$ holds. Again by Lemma 12, we get $\rho(B_{m(n,3)}^*) < 2\sqrt{3} - 1 \cos(n/(2a + 1))$; hence, we have that $\rho(T) < 2\sqrt{3} - 1 \cos(n/(2a + 1))$ holds, where $a = \lceil \log_3(n/3) \rceil + 1$.

4.2. The Comparison of the Results in Theorems 21 and 22. Choose $T \in T_{13}^*$, where $T_{13}^*$ is shown in Figure 19. By Lemma 11, we have that $\rho(T) < 2\sqrt{3} \cos(n/15)$ holds, and by Theorem 22, we get $\rho(T) < 2\sqrt{3} \cos(n/7)$. Obviously, we have that $2\sqrt{3} \cos(n/7) < 2\sqrt{3} \cos(n/15)$ holds; that is, the upper bound of $\rho(T)$ that Theorem 22 gives is better than the one that Theorem 21 gives.

Actually, when $T \in T_{13}^*$ and the length of the only circle in $T$ is 3, the upper bound of $\rho(T)$ that Theorem 22 gives is either equal to the one that Theorem 21 gives or better than the one that Theorem 21 gives.

Choose $T_1 \in T_{13}^*$, where $T_1$ is shown in Figure 20. By Theorem 21, we have that $\rho(T_1) < 2\sqrt{3} \cos(n/15)$ holds, and by Theorem 22, we can get $\rho(T_1) < 2\sqrt{3} \cos(n/7)$. Obviously, we have that $2\sqrt{3} \cos(n/7) < 2\sqrt{3} \cos(n/15)$ holds; that is, the upper bound of $\rho(T)$ that Theorem 22 gives is better than the one that Theorem 21 gives.

Notice that when $T \in T_{13}^*$ and the length of the only circle in $T$ is not less than 4, the upper bound of $\rho(T)$ that Theorem 22 gives may not be better than the one that Theorem 21 gives.

In conclusion, sometimes, the upper bound on the adjacency spectral radius of the unicyclic graphs that Theorem 22 gives is better than the one that Theorem 21 gives.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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