Hindawi
Mathematical Problems in Engineering
Volume 2020, Article ID 9861834, 23 pages
https://doi.org/10.1155/2020/9861834

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

Received 22 March 2020; Accepted 13 June 2020; Published 6 July 2020

Academic Editor: Jean Jacques Loiseau

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 Δ 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 Δ 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 itis 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 graphs [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 of T by $\Delta(T)$. For convenience, we shall sometimes denote $\Delta(T)$ simply by Δ. 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 Δ by T_n^{Δ}.

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 Δ, where $\Delta \geq 3$. Besides, we study the new upper bound on the adjacency spectral radius of unicyclic with n vertices and the maximum degree Δ.

Suppose that $T^* \in T_n^\Delta$, then we obtain some necessary conditions about that T^* is maximal-adjacency-spectrum unicyclic graph in T_n^Δ using the following theorems.

Theorem 1. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, 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 Δ.*

Theorem 2. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ 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 x_{u^*} which corresponds to the vertex u^* in x satisfies that $x_{u^*} = \max_{1\leq i\leq n} x_i$, then $u^* \in V(C)$.*

Theorem 3. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, if the only circle in T^* is C, and there exists a nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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^Δ, let C be the only circle in T^* and $|V(C)| = 3$, if there is no nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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^Δ. If the only circle in T^* is C, there is no nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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^Δ, 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^Δ, 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 $W_1 = \{i|i$ is the leaf node of T^*, and the shortest path from i to r neither pass g_1 nor pass $g_2\}$, $W_2 = \{i|i$ 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 $\max_{i\in W_1} d(i, r) = 1$.

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

If $d(g_2) = 2$, 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 $|d(i, r) - d(j, r)| \leq 1$.

(4) If $W_2 \neq \emptyset$, then $\min_{i\in W_2} d(i, r) \geq \max_{j\in W_1} d(j, r)$.

(5) 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 $\forall j \in W_1$, we all have $d(j, r) = 1$.

Theorem 8. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, $x = (x_1, x_2, \ldots, x_n)^T$ 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^Δ, $x = (x_1, x_2, \ldots, x_n)^T$ 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 $W_1 = \{i|i$ is the leaf node of T^*, and the shortest path from i to r neither pass g_1 nor pass $g_2\}$, $W_2 = \{i|i$ is the leaf node of T^*, and the shortest path from i to r either pass g_1 or pass $g_2\}$. Assume that $T^* \ncong T_{n,2}^\Delta$, 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 (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 $j_1 \in W_2$, which makes (u, j_1) is a pendant edge or $u \in V(C)$ and $d(u) = 2$.

(3) If $\max_{i\in W_1} d(i, r) \neq \min_{i\in W_1} d(i, r)$, 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^Δ if and only if $T^* \cong H_n^\Delta$.*

That is, we describe the structure of the maximal-adjacency-spectrum unicyclic graphs in T_n^{Δ}. 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 Δ 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 $u_1 u_2 \cdots u_k$, where $u_1 = u, k \geq 2, u_k = R$, then we call u_2 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 F to vertex R is FAR, A is a father vertex of F. 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_1 is not equal to the father vertex of w_2, 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 $R\,DM$; 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.

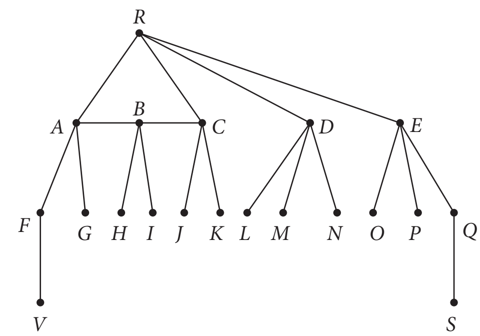

Figure 1: A rooted unicyclic graph.

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 v, w 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 $T^* \in T_n^{\Delta}$, if for any $T \in T_n^{\Delta}$ all have that $\rho(T) \leq \rho(T^*)$ establish, then T^* is called a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}.

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 $T \cong T^{\Delta}_{n,2}$, 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 Δ 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 $T \cong T^{\Delta}_{n,2}$, 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 Δ degree unicyclic graph with levels more than two. Or T is a rooted unicyclic graph obtained from another completely full Δ degree unicyclic graph with levels more than two by deleting some right leaf nodes. Then, T is called an almost completely full Δ degree unicyclic graph. We denote the almost completely full Δ degree unicyclic graph with n vertices and maximum degree Δ by H^{Δ}_n.

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 $T \cong T^{\Delta}_{n,2}$, where $T^{\Delta}_{n,2}$ is shown in Figure 2, and r is the root node of $T^{\Delta}_{n,2}$. Or $T^* \cong T^{\Delta}_{n,3}$, 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 $s + 2 \leq \Delta$), $E(T^{\Delta}_{n,3}) = \{(r, v_1), (r, v_2), (v_1, v_2), (r, v_3), \ldots, (r, v_{\Delta}), (v_1, w_1), \ldots, (v_1, w_s)\}$, 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) $k \geq 3$.

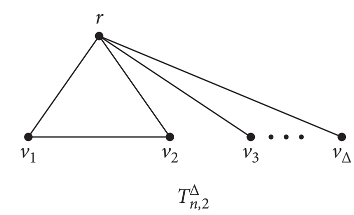

Figure 2: A completely full Δ degree unicyclic graph with levels 2.

(2) 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 $v_1, v_2, \ldots, v_{\Delta}$.
(3) Suppose that the only circle in T is C, and $V(C) = \{r, v_1, v_2\}$.
(4) There is at most one nonfull internal vertex in T.
(5) When there is only one nonfull internal vertex in T, this nonfull internal vertex is in the $k-1$ level of T.

Then, T is an almost full Δ degree unicyclic graph with root node r.

From the definitions above, we know that completely full Δ degree unicyclic graph is the special situation of almost completely full Δ degree unicyclic graph. completely full Δ degree unicyclic graph and almost completely full Δ degree unicyclic graph are both special situations of almost full Δ degree unicyclic graph. For convenience, in this paper, we denote completely full Δ degree unicyclic graph, almost completely full Δ degree unicyclic graph, almost full Δ degree unicyclic graph by completely full-degree unicyclic graph, almost completely full-degree unicyclic graph, and almost full-degree unicyclic graph, respectively.

For instance, suppose that the unicyclic graph shown in Figure 3(a) is a rooted unicyclic graph with root node r, then the rooted unicyclic graph shown in Figure 3(a) is a completely full 3 degree unicyclic graph with levels 3, maximum degree 3, and root node r. Suppose that the root node of the unicyclic graph shown in Figure 3(b) is r, then the rooted unicyclic graph shown in Figure 3(b) is an almost completely full 4 degree unicyclic graph with levels 4, maximum degree 4, and root node r. Suppose that the root node of the unicyclic graph shown in Figure 3(c) is r, then the rooted unicyclic graph shown in Figure 3(c) is an almost full 4 degree unicyclic graph with levels 4, maximum degree 4, and root node r.

In order to give the main results of this paper, we give some lemmas.

2.3. Some Lemmas

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 Δ, $x = (x_1, x_2, \ldots, x_n)^T$ 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 $w \in N_T(v) \backslash u$, let $T_1 = T - (v, w) + (u, w)$, if T_1 is still a simple connected graph, then $\rho(T_1) > \rho(T)$.*

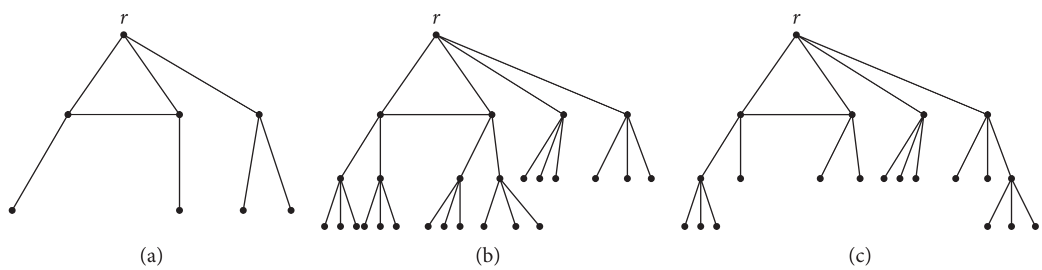

Figure 3: Some unicyclic graphs with roots.

Lemma 2 (see [13]). *Suppose that T is a simple connected graph with n vertices and maximum Δ, $x = (x_1, x_2, \dots, x_n)^T$ 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 $w_1 \in N_T(v)\backslash u, w_2 \in N_T(V)\backslash u, \dots, w_k \in N_T(v)\backslash u$. 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 $\rho(T_1) > \rho(T)$.*

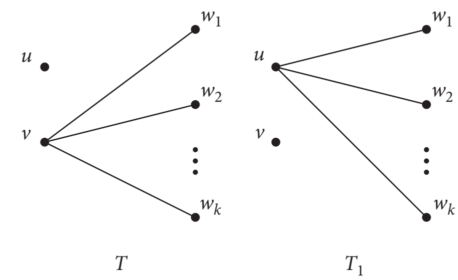

Figure 4: Transition deformation of graphs.

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

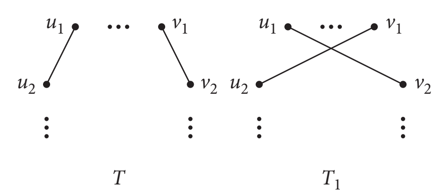

Figure 5: Cross deformation of graphs.

Lemma 4 (see [14]). *Suppose that $T = (V, E)$ is a simple connected graph, and $v_0 v_1 \cdots v_k\ (k \geq 2)$ is an internal path of T. If $T_1 = T - v_{i-1}v_i - v_i v_{i+1} + v_{i-1}v_{i+1}$, where $1 \leq i \leq k-1$, then $\rho(T_1) \geq \rho(T)$.*

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 $V(C) = \{u_1, u_2, \dots, u_l\}$, where $l \geq 4$, and for any natural number i which satisfies $1 \leq i \leq k-1$, we all have $(u_i, u_{i+1}) \in E(T)$, $(u_l, u_1) \in E(T)$, denote $u_{l+1} = u_1, u_{l+2} = u_2, \dots, u_{2l} = u_l$. Suppose that $x = (x_1, x_2, \dots, x_n)^T$ is the Perron vector of T, $\{r_1, r_2, \dots, r_k\}$ (where $1 \leq k \leq l$) is the set which consists of all the vertices whose components of Perron vector are equal to $\max_{1\leq i\leq l} x_{u_i}$ in C, if for any arbitrary natural number j which satisfies $1 \leq j \leq l+1$, we all have $\{u_j, u_{j+1}, \dots, u_{j+k-1}\} \neq \{r_1, r_2, \dots, r_k\}$, 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 $\{u_j, u_{j+1}, \dots, u_{j+k-1}\} \neq \{r_1, r_2, \dots, r_k\}$, we can get $k \geq 2$. Without loss of generality, we assume that $r_1, r_2, \dots, r_k$ 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 $\{u_j, u_{j+1}, \dots, u_{j+k-1}\} \neq \{r_1, r_2, \dots, r_k\}$. We know that there exist two vertices v_1 and v_2 in C and exist two numbers i and s that satisfy both $1 \leq i \leq k-1$, $1 \leq s \leq k$, and $i < s$, which make v_1 is in clockwise arrangement between r_i and r_{i+1}, v_1 is adjacent to r_i, and v_2 is in clockwise arrangement between r_s and r_{s+1}, v_2 is adjacent to r_s, and $x_{v_1} \neq \max_{1\leq i\leq l} x_{u_i}$ and $x_{v_2} \neq \max_{1\leq i\leq l} x_{u_i}$. From the definition of $r_1, r_2, \dots, r_k$, we know $x_{r_i} = x_{r_s} > \max(x_{v_1}, x_{v_2})$. Let $T_1 = T - (r_i, v_1) - (r_s, v_2) + (r_i, r_s) + (v_1, v_2)$, then it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{r_i} > x_{v_2}$ and $x_{r_s} > x_{v_1}$, 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_1, v_2, v_3, and v_4 are four different vertices of T, and $(v_1$ and $v_3) \in E(T)$, $(v_2, v_4) \in E(T)$. If $x = (x_1, x_2, \dots, x_n)^T$ is the Perron vector of T, $x_{v_1}, x_{v_2}, x_{v_3}$, and x_{v_4} correspond to vertices v_1, v_2, v_3, and v_4, respectively, and $x_{v_1} > x_{v_2} > x_{v_3} > x_{v_4}$. Let $T_1 = T - (v_1, v_3) - (v_2, v_4) + (v_1, v_2) + (v_3, v_4)$, if T_1 is still a simple connected graph, then $\rho(T_1) > \rho(T)$.*

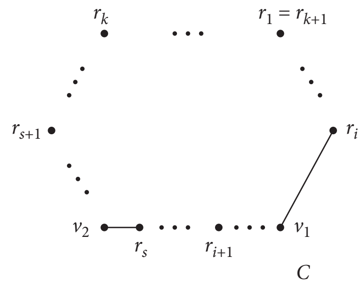

Figure 6: The only circle C in T.

Proof. Since $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of T, we can imply that $\rho(T) = x^T A(T)x$, where $A(T)$ is the adjacency matrix of T. For $x^T A(T_1)x - x^T A(T)x = 2[(x_{v_1} x_{v_2} + x_{v_3}x_{v_4}) - (x_{v_1}x_{v_3} + x_{v_2}x_{v_4})] = 2(x_{v_1} - x_{v_4})(x_{v_2} - x_{v_3}) > 0$, and T_1 is a simple connected graph; hence, we get $\rho(T_1) = \max_{\|y\|=1} y^T A(T_1)y \geq x^T A(T_1)x > x^T A(T)x = \rho(T)$.

Therefore, Lemma 7 holds. □

3. The Properties and Structure of the Maximal-Adjacency-Spectrum Unicyclic Graphs in T_n^Δ

3.1. The Properties of the Maximal-Adjacency-Spectrum Unicyclic Graphs in T_n^Δ. First, we give the properties of the Perron vector of the maximal-adjacency-spectrum unicyclic graphs in T_n^Δ, as in the following theorems:

Theorem 11. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, 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 Δ.*

Proof. Assume that the proposition is not established, we suppose that there exists a vertex v^* in T^* such that $x_{v^*} = \max_{1\leq i\leq n} x_i$ and $d(v^*) < \Delta$. Denote $p = d(v^*)$, it is obvious that $p \geq 2$; hence, $2 \leq p < \Delta$. We choose a vertex u with degree Δ in $V(T^*)$, suppose that $N_{T^*}(u) = \{v_1, v_2, \ldots, v_\Delta\}$. 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 $N_{T^*}(u)\backslash N_{T^*}(v^*)$ such that
$T^* - (u, v_{j_1}) - (u, v_{j_2}) - \cdots - (u, v_{j_{\Delta-p}}) + (v^*, v_{j_1}) + (v^*, v_{j_2}) + \cdots + (v^*, v_{j_{\Delta-p}})$ is still a simple connected graph. Denote
$T_1 = T^* - (u, v_{j_1}) - (u, v_{j_2}) - \cdots - (u, v_{j_{\Delta-p}}) + (v^*, v_{j_1}) + (v^*, v_{j_2}) + \cdots + (v^*, v_{j_{\Delta-p}})$, then it is easy to know $T_1 \in T_n^\Delta$. Again by $x_{v^*} \geq x_u$, 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^Δ; 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^Δ, 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 x_{u^*} which corresponds to the vertex u^* in x satisfies that $x_{u^*} = \max_{1\leq i\leq n} x_i$, then $u^* \in V(C)$.*

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

First, for $\forall v \in V(C)$, we have $x_v > x_{u_k}$. Otherwise, suppose there exists a vertex v_1 in $V(C)$ such that $x_{v_1} \leq x_{u_k}$. Now according to the value of $d(v_1)$, we discuss the following two cases:

Case 1. $d(v_1) < \Delta$.

Since $v_1 \in V(C)$, we have $|N_{T^*}(v_1)| \geq 2$; thus in the set of $V(T^*)$, there exists a vertex v_2 which satisfies $v_2 \in N_{T^*}(v_1)$ such that $T^* - (v_2, v_1) + (v_2, u_k)$ is still a simple connected graph. Denote $T_1 = T^* - (v_2, v_1) + (v_2, u_k)$, then it is easy to know $T_1 \in T_n^\Delta$. By Lemma 1, we get $\rho(T_1) > \rho(T^*)$, and this implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ.

Case 2. $d(v_1) = \Delta$.

In this case, it is easy to know that in the set of $N_{T^*}(v_1)$, there exist $\Delta - 1$ vertices $v_2, v_3, \ldots, v_\Delta$ such that $T^* - (v_1, v_2) - (v_1, v_3) - \cdots - (v_1, v_\Delta) + (u_k, v_2) + (u_k, v_3) + \cdots + (u_k, v_\Delta)$ is still a simple connected graph. Denote $T_1 = T^* - (v_1, v_2) - (v_1, v_3) - \cdots - (v_1, v_\Delta) + (u_k, v_2) + (u_k, v_3) + \cdots + (u_k, v_\Delta)$, then it is easy to know $T_1 \in T_n^\Delta$. From $x_{v_1} \leq x_{u_k}$, by Lemma 2, 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^Δ.

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 $x_v > x_{u_k}$ holds.

Second, denote u^* by u_0, suppose that v is the vertex which is nearest to u^* in C. Choose two vertices v_1 and v_2 different from v in C, then $x_{u_0} \geq x_{v_1}, x_{u_0} \geq x_{v_2}, x_{v_1} > x_{u_k}$, and $x_{v_2} > x_{u_k}$. 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 $x_{v_1} \leq x_{u_{l-1}}, x_{v_2} > x_{u_l}$ and ② $x_{v_2} \leq x_{u_{l-1}}, x_{v_1} > x_{u_l}$ holds. Without loss of generality, we assume that there exists a natural number l which satisfies $1 \leq l \leq k$ such that $x_{v_1} \leq x_{u_{l-1}}$ and $x_{v_2} > x_{u_l}$. Then, let $T_2 = T^* - (u_{l-1}, u_l) - (v_1, v_2) + (v_2, u_{l-1}) + (v_1, u_l)$, 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^Δ. Therefore, Theorem 12 holds. □

Lemma 8. *Assume that $T \in T_n^{\Delta}$, $x = (x_1, x_2, \ldots, x_n)^T$ 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 $x_{u_1} = x_{u_2} = \cdots = x_{u_l}$, then there must exist $T_1 \in T_n^{\Delta}$ 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^{Δ}. From Theorem 12, we can get $x_{u_1} = x_{u_2} = \cdots = x_{u_l} = \max_{1 \leq i \leq n} x_i$; again by Theorem 11, we get $d(u_1) = d(u_2) = \cdots = d(u_l) = \Delta \geq 3$; hence, for any natural number i which satisfies $1 \leq i \leq l$, and we all have $N_T(u_i) \backslash V(C) \neq \varnothing$. Besides, from Theorem 12, we get that for $\forall v \in V(T) \backslash V(C)$, 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 $N_T(u_1) \backslash V(C) \neq \varnothing$, choose $v \in N_T(u_1) \backslash V(C)$, then we have $x_v < x_{u_1}$. For $l \geq 4$, we can know u_1, v, u_{l-1}, andu_l are different from each other. From $x_{u_1} = x_{u_2} = \cdots = x_{u_l}$ and $x_{u_1} > x_v$, we know that $x_{u_{l-1}} = x_{u_1} > x_v$; again from $x_{u_1} = x_{u_l}$, we can get $x_{u_1} \geq x_{u_l}$. Let $T_1 = T - (u_1, v) - (u_l, u_{l-1}) + (u_1, u_{l-1}) + (u_l, v)$, then it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{u_{l-1}} > x_v$ and $x_{u_1} \geq x_{u_l}$, 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^{Δ}. Therefore, Lemma 8 holds. □

Lemma 9. *Assume that $T \in T_n^{\Delta}$, where $T = (V(T), E(T))$, C is the circle of T, $V(C) = \{u_1, u_2, \ldots, u_l\}, l \geq 4$, and for any natural number i which satisfies $1 \leq i \leq l - 1$, we all have $(u_i, u_{i+1}) \in E(T)$, $(u_l, u_1) \in E(T)$. 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 $T_1 \in T_n^{\Delta}$ 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^{Δ}.

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 $u_{l+1} = u_1$, 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 $(u_l, u_1) \in E(T)$; 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 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 $1 \leq t \leq l - m + 1$ 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 $V(T_1) = V(T) \backslash \{u_{t+1}\}$ and $E(T_1) = E(T) - (u_t, u_{t+1}) - (u_{t+1}, u_{t+2}) + (u_t, u_{t+2})$. It is easy to know $T_1 \in T_{n-1}^{\Delta}$, and by Lemma 4, we have that $\rho(T_1) \geq \rho(T)$ holds.

Suppose that v_1 is an arbitrary leaf node of T_1. Let $T_2 = T_1 + (v_1, u_{t+1})$, then it is easy to know $T_2 \in T_n^{\Delta}$, 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^{Δ}.

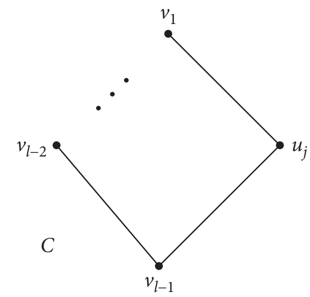

Figure 7: Vertex permutation graph of cycle C.

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 $V(C) = \{v_1, v_2, \ldots, v_{l-1}, u_j\}$, 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 $x_{u_j} > \max\{x_{v_1}, x_{v_2}, \ldots, x_{v_{l-1}}\}$. From $l \geq 4$, we know that v_{l-2}, v_{l-1}, and v_1 are different. And for $x_{u_j} > x_{v_{l-1}}$, it is easy to prove that $x_{v_1} > x_{v_{l-2}}$ holds. Otherwise, $x_{v_1} \leq x_{v_{l-2}}$, let $T_1 = T - (v_{l-1}, v_{l-2}) - (u_j, v_1) + (u_j, v_{l-2}) + (v_1, v_{l-1})$, then it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{u_j} > x_{v_{l-1}}$ and $x_{v_{l-2}} \geq x_{v_1}$, 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^{Δ}; hence, $x_{v_1} > x_{v_{l-2}}$. Let $T_2 = T - (v_{l-1}, v_{l-2}) + (v_{l-1}, v_1)$, then it is easy to know $T_2 \in T_n^{\Delta}$, 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^{Δ}.

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^{Δ}, 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 $x_i < x_j$ holds, 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^{Δ}, 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 $\max_{1 \leq l \leq n} x_l$ 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 $x_u \geq x_i$ holds. Otherwise, there exists a vertex w which is not the vertex j_0 and is not a leaf node i_1 in T^*, which makes $x_w < x_{i_1}$. For w is not the leaf node, hence $d(w) \geq 2$, thus there exists a vertex v in the set of $N_{T^*}(w)$ such that $T^* - (v, w) + (v, i_1)$ still belong to T_n^{Δ}. Let

$T_1 = T^* - (v, w) + (v, i_1)$, then by Lemma 1, we have that $\rho(T_1) > \rho(T)$ holds, this implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ. Again since $x_{j_0} = \max_{1\le l\le n} x_l$, then $x_{j_0} \ge x_u$; thus, for any vertex j which is not the leaf node in T^*, and for any leaf node i in T^*, we all have that $x_j > x_i$ holds.

For the properties of the nonfull internal vertices of the maximal-adjacency-spectrum unicyclic graph in T_n^Δ, we have the following theorems. □

Theorem 13. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, if the only circle in T^* is C, and there exists a nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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^Δ, the only circle in T^* is C, there exists a nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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 $u_1 \in V(T^*)\backslash V(C)$.

Let $x = (x_1, x_2, \ldots, x_n)^T$ be the Perron vector of T^*, x_{u_1} and x_{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. $x_{u_1} \ge x_{u_2}$.

Since u_2 is the nonfull internal vertex in T^*, then $N_{T^*}(u_2)\backslash u_1 \ne \varnothing$, choose $w \in N_{T^*}(u_2)\backslash u_1$. Let $T_1 = T^* - (w, u_2) + (w, u_1)$, 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^Δ.

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

Since u_1 is the nonfull internal vertex in T^*, then $N_{T^*}(u_1)\backslash u_2 \ne \varnothing$, choose $w \in N_{T^*}(u_1)\backslash u_2$. 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 $\rho(T_1) > \rho(T^*)$ holds, and this implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ.

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 $|N_{T^*}(u_1)\backslash N_{T^*}(u_2)| \ge 1$ and $|N_{T^*}(u_2)\backslash N_{T^*}(u_1)| \ge 1$ 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. $x_{u_1} \le x_{u_2}$.

Since $|N_{T^*}(u_1)\backslash N_{T^*}(u_2)| \ge 1$ and T^* is a unicyclic graph, we know that there exists $w \in N_{T^*}(u_1)\backslash N_{T^*}(u_2)$ 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^Δ.

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

For $|N_{T^*}(u_2)\backslash N_{T^*}(u_1)| \ge 1$ and T^* is a unicyclic graph, we know that there exists $w \in N_{T^*}(u_2)\backslash N_{T^*}(u_1)$ 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^Δ.

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^Δ, let C be the only circle in T^*, and $|V(C)| = 3$, if there is no nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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 $x_v = \max_{1\le i\le n} x_i$, 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 $d(u_1) \ne 2$ and $d(u_2) \ne 2$, then we must have that $d(u_1) \ge 3$ and $d(u_2) \ge 3$ hold. Hence, $N_{T^*}(u_1)\backslash V(C) \ne \varnothing$ and $N_{T^*}(u_2)\backslash V(C) \ne \varnothing$. Choose $s_1 \in N_{T^*}(u_1)\backslash V(C)$, $s_2 \in N_{T^*}(u_2)\backslash V(C)$. Without loss of generality, we assume that $x_{u_1} \ge x_{u_2}$, and let $T_1 = T^* - (u_2, s_2) + (s_2, u_1)$, 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^Δ. 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^Δ. For the length of the circle of the maximal-adjacency-spectrum unicyclic graphs in T_n^Δ, we have the following theorems.

Theorem 15. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ. If the only circle in T^* is C, there is no nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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^Δ, the only circle in T^* is C, there is no nonfull internal vertex in the set of $V(T^*)\backslash V(C)$, 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_{u_1} and x_{u_2} 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 $u_1 v_1 v_2 \cdots v_k u_2$ which satisfies $k \geq 2$ in C. Without loss of generality, we assume that $x_{u_1} \geq x_{u_2}$. Let $T_1 = T^* - (v_k, u_2) + (v_k, u_1)$, 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^Δ.

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 $u_1 v_1 v_2 u_2$ in C. Without loss of generality, we assume that $x_{u_1} \geq x_{u_2}$. Let $T_1 = T^* - (v_2, u_2) + (v_2, u_1)$, 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^Δ.

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 $d(v_1) = d(w_1) = \Delta$ 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 $v_1, w_1, u_1,$ and 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 $d(v_1) = d(w_1) = \Delta \geq 3$, we have that $v_1 u_1 w_1$ is an internal path, let $T_1 = (V(T_1), E(T_1))$, where $V(T_1) = V(T^*)\backslash\{u_1\}, E(T_1) = E(T^*) - (v_1, u_1) - (u_1, w_1) + (v_1, w_1)$, then it is easy to know $T_1 \in T_{n-1}^\Delta$. By Lemma 4, we have that $\rho(T_1) \geq \rho(T^*)$ 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 $T_2 \in T_n^\Delta$. 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^Δ.

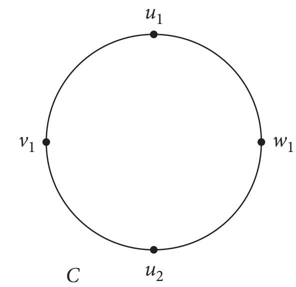

Figure 8: Vertex permutation graph of cycle C with four vertices.

From $d(u_1) \geq 3$ and $d(u_2) \geq 3$, we know that $N_{T^*}(u_1)\backslash V(C) \neq \varnothing$ and $N_{T^*}(u_2)\backslash V(C) \neq \varnothing$ hold. Choose $s_1 \in N_{T^*}(u_1)\backslash V(C)$ and $s_2 \in N_{T^*}(u_2)\backslash V(C)$. Without loss of generality, assume that $x_{u_1} \geq x_{u_2}$. Let $T_3 = T^* - (s_2, u_2) + (s_2, u_1)$, then it is easy to know $T_3 \in T_n^\Delta$. 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^Δ.

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^Δ, 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^Δ and C is the only circle in T^*. Denote $|V(C)| = l$; 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 most one nonfull internal vertex in T^*. Suppose that $V(C) = \{u_1, u_2, \ldots, u_l\}$, and $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of T^*. By Theorem 12, we can get $\max_{1\leq i\leq l} x_{u_i} = \max_{1\leq i\leq n} x_i$. Then, from $l \geq 4$, T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, and from Lemma 8, we can know $\max_{1\leq i\leq l} x_{u_i} > \min_{1\leq i\leq l} x_{u_i}$. 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 $\max_{1\leq i\leq 4} x_{u_i} = \max_{1\leq j\leq n} x_j$ holds. Without loss of generality, assume that $x_{u_1} = \max_{1\leq i\leq 4} x_{u_i}$, then we have $x_{u_1} = \max_{1\leq j\leq n} x_j$; again from Theorem 11, we can get $d(u_1) = \Delta\,(\Delta \geq 3)$. Without loss of generality, we assume that $u_1, u_2, u_3,$ and u_4 have anticlockwise arrangement in C, and the position of the relationship of these vertices is shown in Figure 9.

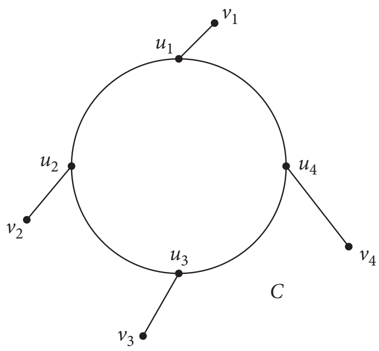

Figure 9: Cycle C with four vertices.

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

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

For there is at most one nonfull internal vertex in T^*, there is at most one of $d(u_2), d(u_3)$, and$d(u_4)$ unequal to Δ $(\Delta \ge 3)$. Besides, $\min\{d(u_2), d(u_3), d(u_4)\} \ge 3$; otherwise, $\min\{d(u_2), d(u_3), d(u_4)\} = 2$. 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 $V(T_1) = V(T^*)\backslash\{q_2\}, E(T_1) = E(T^*) - (q_1, q_2) - (q_2, q_3) + (q_1, q_3)$. Then, it is easy to know $T_1 \in T^{\Delta}_{n-1}$, and by Lemma 4, we have that $\rho(T_1) \ge \rho(T^*)$ 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 $T_2 \in T^{\Delta}_n$. 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^{Δ}_n. Then, we have $\min\{d(u_2), d(u_3), d(u_4)\} \ge 3$, and $\min_{1\le i\le 4} d(u_i) \ge 3$. Therefore, for any vertex u_i which satisfies $1 \le i \le 4$ in the set of $V(C)$, we all have that $N_{T^*}(u_i)\backslash V(C) \neq \varnothing$ holds.

Proposition 2. $x_{u_3} = \min\{x_{u_2}, x_{u_3}, x_{u_4}\}$.

Assume that $x_{u_3} = \min\{x_{u_2}, x_{u_3}, x_{u_4}\}$ is not established, and we have $x_{u_3} > \min\{x_{u_2}, x_{u_3}, x_{u_4}\}$. Without loss of generality, assume that $\min\{x_{u_2}, x_{u_3}, x_{u_4}\} = x_{u_2}$, then we have $x_{u_3} > x_{u_2}$. Let $T_1 = T^* - (u_1, u_2) - (u_3, u_4) + (u_1, u_3) + (u_2, u_4)$, then it is easy to know $T_1 \in T^{\Delta}_n$. From $x_{u_1} \ge x_{u_4}$ and $x_{u_3} > x_{u_2}$, 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^{Δ}_n; hence, the hypothesis is not established. Therefore, $x_{u_3} = \min\{x_{u_2}, x_{u_3}, x_{u_4}\}$.

Proposition 3. *For $\forall v \in N_{T^*}(u_2)\backslash V(C)$, we all have that $x_{u_4} = x_v$ holds.*

And for $\forall w \in N_{T^*}(v_4)\backslash V(C)$, we all have that $x_w = x_{u_2}$ holds. From Proposition 1, we know $N_{T^*}(u_2)\backslash V(C) \neq \varnothing$. Assume that, for $\forall v \in N_{T^*}(u_2)\backslash V(C)$, we all have that the proposition $x_{u_4} = x_v$ is not established, then there must exists a vertex $v_2 \in N_{T^*}(u_2)\backslash V(C)$ such that $x_{u_4} \neq x_{v_2}$.

Proposition 4. *$d(u_2) = \Delta$ and $d(u_4) = \Delta$.*

If $d(u_2) = \Delta$ is not established, then $d(u_2) < \Delta$. From Proposition 1, we know $N_{T^*}(u_3)\backslash V(C) \neq \varnothing$. Choose $v_3 \in N_{T^*}(u_3)\backslash V(C)$, and let $T_1 = T^* - (v_3, u_3) + (v_3, u_2)$, then it is easy to know $T_1 \in T^{\Delta}_n$. From Proposition 2, we know $x_{u_3} \le x_{u_2}$, 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^{Δ}_n. Hence, the hypothesis is not established, that is, $d(u_2) = \Delta$. The same reason, we can prove that $d(u_4) = \Delta$ holds.

Proposition 5. $x_{u_4} = x_{u_2}$.

From Proposition 1, we know $N_{T^*}(u_2)\backslash V(C) \neq \varnothing$ and $N_{T^*}(u_4)\backslash V(C) \neq \varnothing$. For $Ax = \rho(T^*)x$, where A is the adjacency matrix of T^*, denote $\rho = \rho(T^*)$, then $\rho x_{u_4} = x_{u_1} + x_{u_3} + \sum_{p\in N_{T^*}(u_4)\backslash} V(C) x_p, \rho x_{u_2} = x_{u_1} + x_{u_3} + \sum_{q\in N_{T^*}} (u_2)\backslash V(C) x_q$. From Propositions 3 and 4, we can know $\sum_{p\in N_{T^*}(u_4)\backslash V(C)} x_p = (\Delta - 2)x_{u_2}$ and $\sum_{q\in N_{T^*}(u_2)\backslash V(C)} x_q = (\Delta - 2)x_{u_4}$; thus, we have $\rho x_{u_4} = x_{u_1} + x_{u_3} + (\Delta - 2)x_{u_2}$ and $\rho x_{u_2} = x_{u_1} + x_{u_3} + (\Delta - 2)x_{u_4}$. Hence, $(\rho + \Delta - 2)$ $(x_{u_4} - x_{u_2}) = 0$. Therefore, $x_{u_4} = x_{u_2}$.

Proposition 6. $x_{u_1} = x_{u_2}$ *and* $x_{u_1} = x_{u_4}$.

Assume that $x_{u_1} \neq x_{u_2}$, then from $x_{u_1} = \max_{1\le i\le 4} x_{u_i}$, we know $x_{u_1} > x_{u_2}$. From Proposition 1, we can get $N_{T^*}(u_2)\backslash V(C) \neq \varnothing$. Choose $v_2 \in N_{T^*}(u_2)\backslash V(C)$, let $T_1 = T^* - (u_1, u_4) - (u_2, v_2) + (v_2, u_1) + (u_2, u_4)$, and then it is easy to know $T_1 \in T^{\Delta}_n$. From Proposition 3, we know $x_{v_2} = x_{u_4}$; hence, $x_{u_4} \le x_{v_2}$. And for $x_{u_1} > x_{u_2}$, 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^{Δ}_n; hence, we have that $x_{u_1} = x_{u_2}$ holds. And from Proposition 5, we get $x_{u_4} = x_{u_2}$; therefore, $x_{u_1} = x_{u_4}$.

From Proposition 2, we know $x_{u_3} = \min\{x_{u_2}, x_{u_3}, x_{u_4}\}$; from Proposition 6, we have $x_{u_1} = x_{u_2} = x_{u_4}$, and by Lemma 8, we know $\max_{1\le i\le 4} x_{u_i} > \min_{1\le i\le 4} x_{u_i}$; hence, $x_{u_3} < x_{u_4}$. Let $T_2 = T^* - (u_1, u_4) - (u_2, u_3) + (u_3, u_1) + (u_2, u_4)$, then it is easy to know $T_2 \in T^{\Delta}_n$. From $x_{u_3} < x_{u_4}$ and $x_{u_1} \le x_{u_2}$, 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^{Δ}_n.

Therefore, in conclusion, case 1 implies a contradiction.

Case 2. $l \ge 5$.

In this case, from Lemma 8, we have that $\min_{1\le i\le l} x_{u_i} < \max_{1\le i\le l} x_{u_i}$. Let s be a vertex in C such that $x_s = \min_{1\le i\le l} x_{u_i}$. From Theorem 12, we can get that there exists a natural number i_0 which satisfies $1 \le i_0 \le l$ such that $x_{u_{i_0}} = \max_{1\le i\le n} x_i$. Assume that k is the number of the vertices whose components are equal to $\max_{1\le i\le n} x_i$ in C. From $\min_{1\le i\le l} x_{u_i} < \max_{1\le i\le l} x_{u_i}$, we have $l - k \ge 1$. Suppose that $r_1, r_2, \ldots, r_k$ are all the vertices whose components are equal to $\max_{1\le i\le n} x_i$ 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 $s, \ldots, r_1, r_2, \ldots, r_k, \ldots, s$ in sequence.

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

Assume that $k \ge 2$ is not established, then $k = 1$. Then now, 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

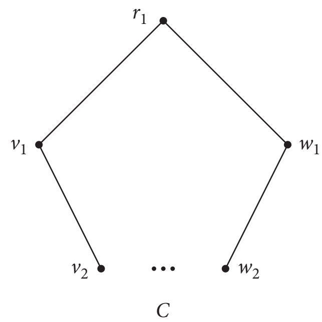

FIGURE 10: Vertex permutation graphs of cycle C with no less than 5 vertices.

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 i which satisfies* $1 \le i \le 2$, *we all have that* $x_{v_i} < x_{r_1}$ *and* $x_{w_i} < x_{r_1}$ *hold.*

From Lemma 9, we can get $N_{T^*}(w_1)\backslash V(C) \neq \varnothing$. *Then for* $\forall t \in N_{T^*}(w_1)\backslash V(C)$, *we all have that* $x_t < x_{v_1}$ *holds. Otherwise, there exists* $t_1 \in N_{T^*}(w_1)\backslash V(C)$ *such that* $x_{t_1} \ge x_{v_1}$. *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* $T_1 \in T_n^{\Delta}$. *From* $x_{t_1} \ge x_{v_1}$ *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^{Δ}.

Besides, we also can prove $x_{v_2} < x_{w_1}$. *Otherwise,* $x_{v_2} \ge x_{w_1}$; *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* $T_2 \in T_n^{\Delta}$. *From* $x_{v_2} \ge x_{w_1}$ *and* $x_{v_1} < x_{r_1}$, *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^{Δ}.

Choose $t_2 \in N_{T^*}(w_1)\backslash V(C)$; *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* $T_3 \in T_n^{\Delta}$. *From the above conclusion, we have* $x_{t_2} < x_{v_1}$. *For* $x_{v_2} < x_{w_1}$, *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^{Δ}. *Hence, the hypothesis is not established; therefore,* $k \ge 2$ *holds.*

Second, we can prove that $l - k \ge 2$ *holds.*

Assume that $l - k \ge 2$ *is not established, then* $l - k = 1$; *hence, we can suppose that the vertices which follow the clockwise direction in C are* $s, r_1, r_2, \ldots, r_k$ *in sequence. From* $l \ge 5$, *we know that* $k \ge 4$ *holds; thus* s, 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* $T_4 \in T_n^{\Delta}$. *From the definitions of* $r_1, r_2, \ldots, r_k$ *and s, we know* $x_s < x_{r_k}$. *Since* $x_{r_1} \ge x_{r_{k-1}}$, *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^{Δ}. *Therefore,* $l - k = 1$ *is not established, then we have* $l - k \ge 2$.

Denote $m = l - k$, *from* $l - k \ge 2$, *and we have that* $m \ge 2$ *holds. Then, we can suppose that the vertices which follow the clockwise direction in C are* $v_m, \ldots, v_1, r_1, \ldots, r_k$ *in sequence. From* $m \ge 2$ *and* $k \ge 2$, *we know that* v_m, 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.*

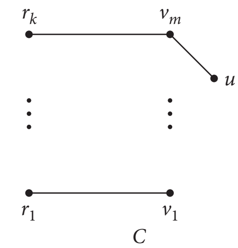

FIGURE 11: The relationship of the vertices of C.

For the relationship between x_{v_1} *and* x_{v_m}, *we must have that* $x_{v_1} = x_{v_m}$ *holds. Otherwise, there must exist one of the two equations,* $x_{v_1} < x_{v_m}$ *and* $x_{v_1} > x_{v_m}$, *holds. Let* $T_5 = T^* - (r_1, v_1) - (r_k, v_m) + (r_1, v_m) + (v_1, r_k)$, *then it is easy to know* $T_5 \in T_n^{\Delta}$. *If* $x_{v_1} < x_{v_m}$, *for* $x_{r_1} \ge x_{r_k}$, *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^{Δ}. *If* $x_{v_1} > x_{v_m}$, *for* $x_{r_1} \le x_{r_k}$, *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^{Δ}. *Hence,* $x_{v_1} = x_{v_m}$. *Then, we have that* $x_{v_m} \ge x_{v_1}$ *holds.*

By Lemma 9, we know $d(v_m) \ge 3$; *hence,* $N_{T^*}(v_m)\backslash V(C) \neq \varnothing$. *Choose* $u \in N_{T^*}(v_m)\backslash V(C)$; *then from Theorem 11, we get* $x_u < x_{r_1}$. *Let* $T_6 = T^* - (r_1, v_1) - (u, v_m) + (r_1, v_m) + (v_1, u)$, *it is easy to know* $T_6 \in T_n^{\Delta}$. *From* $x_{v_m} \ge x_{v_1}$ *and* $x_u < x_{r_1}$, *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^{Δ}.

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 $l \ge 5$, a contradiction is implied. Hence, $l \ge 4$ 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^{Δ}, 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^{Δ}, *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* $W_1 = \{i | i$ *is the leaf node of* T^*, *and the shortest path from i to r neither pass* g_1 *nor pass* $g_2\}$, $W_2 = \{i | i$ *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* $W_2 = \varnothing$, *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* $|1 - d(i, r)| \le 1$.

If $d(g_2) = 2$, *then for the arbitrary leaf node i in* T^*, *we all have* $|1 - d(i, r)| \le 1$.

(3) *If* $W_2 \neq \varnothing$, *then for the arbitrary leaves i, j in* T^*, *we all have* $|d(i, r) - d(j, r))| \le 1$.

(4) *If* $W_2 \neq \varnothing$, *then* $\min_{i\in W_2} d(i,r) \geq \max_{j\in W_1} d(j,r)$.

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

Proof. Assume that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}, 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 $\max_{i\in W_1} d(i,r) = 1$ 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 $u_1u_2\cdots u_k r$, where $u_1 = i, k \geq 2$. By Lemma 1, it is easy to prove that $x_{g_1} < x_{u_2}$ holds. And from Lemma 10, we get $x_{g_2} > x_{u_1}$. Let $T_1 = T^* - (g_1, g_2) - (u_1, u_2) + (u_2, g_2) + (g_1, u_1)$, it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{g_1} < x_{u_2}$ and $x_{g_2} > x_{u_1}$, 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^{Δ}. Hence, $\max_{i\in W_1} d(i,r) = 1$.

Therefore, (1) of Theorem 17 holds.

(2) Assume that $d(g_1) = 2$, 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 $rv_1v_2\cdots v_k$, where $v_k = i$. From $|1 - d(i,r)| > 1$, we know $d(i,r) \geq 3$, then we have $k \geq 3$. Let $T_1 = T^* - (v_{k-1}, v_k) + (g_1, v_k)$, then it is easy to know $T_1 \in T_n^{\Delta}$. If $x_{g_1} \geq x_{v_{k-1}}$, then 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^{Δ}; 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 $T_2 \in T_n^{\Delta}$. Since $x_{g_1} < x_{v_{k-1}}$, and from Lemma 10, we know that $x_{v_k} < x_r$ holds. 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^{Δ}. Hence, when $d(g_1) = 2$, for any leaf node i in T^*, we all have that $|1 - d(i,r)| \leq 1$ holds. Similarly, when $d(g_2) = 2$, for any leaf node i in T^*, we all 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 $l \geq 1$ hold. 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 $rv_kv_{k-1}\cdots v_2v_1$ and the path P_2 by $ru_l\cdots u_2u_1$, where $v_1 = i$ and $u_1 = j$; P_1 and P_2 are shown in Figure 12. Besides, we denote $u_{l+1} = r$; by the definition of r, we know $x_{u_{l+1}} \geq x_{v_k}$. For u_1 is the leaf node in T^* and v_2 is the nonleaf node in T^*, then by Lemma 10, we have $x_{u_1} < x_{v_2}$.

From $x_{u_1} < x_{v_2}, x_{u_{l+1}} \geq x_{v_k}$ and $k - 1 \geq l + 1$, we know that there exists a natural number s that satisfies $1 \leq s \leq l$, which make $x_{u_s} < x_{v_{s+1}}$ and $x_{u_{s+1}} \geq x_{v_{s+2}}$. Let $T_1 = T^* - (u_s, u_{s+1}) - (v_{s+1}, v_{s+2}) + (v_{s+1}, u_{s+1}) + (u_s, v_{s+2})$, then it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{u_s} < x_{v_{s+1}}$ and $x_{u_{s+1}} \geq x_{v_{s+2}}$, 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^{Δ}.

Case 2. There is a public edge between P_1 and P_2.

From that $W_2 \neq \varnothing, \Delta \geq 3$, 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 $k = 2 + l$. Otherwise, $k > 2 + l$, it will imply that the difference in lengthen 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 $u_0u_1u_2\cdots u_{t+1}\cdots r$ and P_2 is $v_2v_3\cdots v_{t+1}\cdots r$, where $u_0 = i, v_2 = j$, and there exists $t \geq 2$ such that, for $\forall j \geq t+1$, we all have $u_j = v_j$. Let P_3 be $w_1w_2w_3\cdots w_{t+1}\cdots r$, where w_1 is denoted by w, and denote $u_k = r$.

Now, we consider the paths P_1 and P_3.

For w_1 is the leaf node in T^* and u_1 is the nonleaf node in T^*, then by Lemma 10, we get $x_{w_1} < x_{u_1}$. If there exists a natural number s that satisfies $1 \leq s \leq t$, which make that both $x_{w_s} < x_{u_s}$ and $x_{w_{s+1}} \geq x_{u_{s+1}}$ hold. Let $T_1 = T^* - (w_s, w_{s+1}) - (u_s, u_{s+1}) + (w_{s+1}, u_s) + (u_{s+1}, w_s)$, then it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{w_s} < x_{u_s}$ and $x_{w_{s+1}} \geq x_{u_{s+1}}$, 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^{Δ}. Hence, for any natural number s which satisfies $1 \leq s \leq t$, $x_{w_s} < x_{u_s}$, and $x_{w_{s+1}} \geq x_{u_{s+1}}$ cannot hold meanwhile. And for $x_{w_1} < x_{u_1}$, then we have that, for any natural number s which satisfies $1 \leq s \leq t+1$, we all have $x_{w_s} < x_{u_s}$.

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 $x_{v_{t+1}} = x_{u_{t+1}} > x_{w_{t+1}}$, then there exists a natural

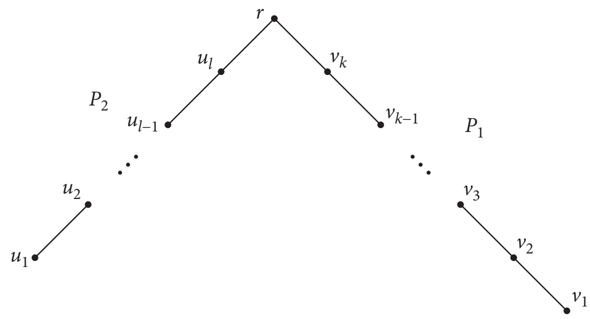

Figure 12: A graph with no common edge between two paths.

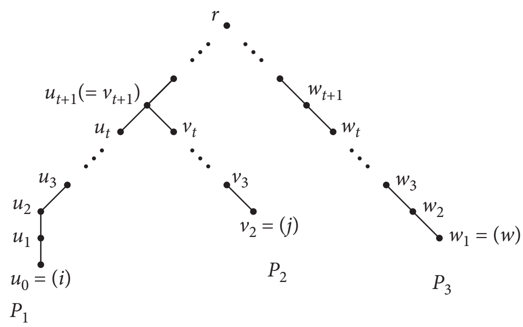

Figure 13: A graph with common edge(s) between two paths.

number s that satisfies $2 \le s \le t$, which make that both $x_{v_s} < x_{w_s}$ and $x_{v_{s+1}} \ge x_{w_{s+1}}$ hold. Let $T_2 = T^* - (v_s, v_{s+1}) - (w_s, w_{s+1}) + (w_{s+1}, v_s) + (v_{s+1}, w_s)$, then it is easy to know $T_2 \in T_n^\Delta$. From $x_{v_s} < x_{w_s}$ and $x_{v_{s+1}} \ge x_{w_{s+1}}$, by Lemma 3, we know that $\rho(T_2) > \rho(T^*)$ holds, and this implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ.

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 $d(i,r) \ge 2$. Without loss of generality, we assume that the shortest path from r to i is $rv_1v_2 \cdots v_s$ and the shortest path from r to j is $rw_1w_2 \cdots w_k$, where $i = v_s$ and $j = w_k$. Then, we have that $k > s$ and $s \ge 2$ 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 $T_1 = T^* - (v_{s-1}, v_s) - (w_{k-1}, w_{k-2}) + (w_{k-1}, v_{s-1}) + (v_s, w_{k-2})$, it is easy to know $T_1 \in T_n^\Delta$. From $x_{w_{k-1}} > x_{v_s}$, if $x_{w_{k-2}} \le x_{v_{s-1}}$, then by Lemma 3, we have that $\rho(T_1) > \rho(T^*)$ holds. This implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ; hence, $x_{w_{k-2}} > x_{v_{s-1}}$. By mathematical induction, we get $x_{w_{k-s}} > x_{v_{s-(s-1)}}$, then we have that $x_{w_1} > x_{v_1}$ holds.

We also can prove that $x_{w_2} > x_{g_2}$ holds. Otherwise, $x_{w_2} \le x_{g_2}$. For $x_{w_1} > x_{v_1}$, let $T_2 = T^* - (w_1, w_2) - (v_1, g_2) + (w_1, g_2) + (v_1, w_2)$, it is easy to know $T_2 \in T_n^\Delta$. From $x_{w_2} \le x_{g_2}$ and $x_{w_1} > x_{v_1}$, 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^Δ. Let $T_3 = T^* - (w_1, w_2) + (w_1, g_2) + (r, w_2)$, it is easy to know $T_3 \in T_n^\Delta$. From $x_r \ge x_{w_1}$ and $x_{w_2} > x_{g_2}$, 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^Δ.

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 $W_2 \ne \varnothing$, 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 $W_2 \ne \varnothing$, 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 $d(i,r) \ge 3$. Suppose that the shortest path from i to r is $v_1v_2 \cdots v_kr$, where $v_1 = i$. Then, from $d(i,r) \ge 3$, we know that $k \ge 3$ holds, and from $d(g_2) = 2$, we know that $v_k = g_1$ holds. Let $T_1 = T^* - (v_1, v_2) - (r, g_2) + (r, v_2) + (g_2, v_1)$, from $v_k = g_1$ and $k \ge 3$, we know $T_1 \in T_n^\Delta$. And by Lemma 1, it is easy to prove $x_{v_2} > x_{g_2}$. For $x_{v_1} \le x_r$, 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^Δ; hence, the hypothesis is not established. Therefore, T^* is a rooted unicyclic graph with levels 3.

Next, we prove that, for $\forall j \in W_1$, we all have $d(j,r) = 1$. Otherwise, assume that there exists a vertex $j_0 \in W_1$ such that $d(j_0, r) \ge 2$. 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_1w_2r, 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 that $x_{g_2} \le x_{w_2}$ holds. By Lemma 10, we can get $x_{g_1} > x_{w_1}$. Let $T_2 = T^* - (g_1, g_2) - (w_1, w_2) + (g_1, w_2) + (g_2, w_1)$, then it is easy to know $T_2 \in T_n^\Delta$. From $x_{g_2} \le x_{w_2}$ and $x_{g_1} > x_{w_1}$, 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^Δ. Hence, the hypothesis is not established. Therefore, for $\forall j \in W_1$, 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_n^Δ and the almost full-degree unicyclic graphs, we have the following theorem. □

Theorem 18. *Suppose that T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^Δ, $x = (x_1, x_2, \ldots, x_n)^T$ 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 $r \in V(C)$, then let $V(C) = \{r, g_1, g_2\}$. Denote $W_1 = \{i | i$ is the leaf node of T^*, and the shortest path from i to r neither pass g_1 nor pass $g_2\}$, $W_2 = \{i | i$ is the leaf node of T^*, and the shortest path from i to r either pass g_1 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 the 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 $W_2 = \varnothing$; by (1) of Theorem 17, we know $\max_{i \in W_1} d(i, r) = 1$; thus, $T^* \cong T_{n,2}^\Delta$, where $T_{n,2}^\Delta$ 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 $W_2 \neq \varnothing$. 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 $\forall j \in W_1$, we all 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_2 is the nonfull internal vertex in C, then we have that $d(g_1) = \Delta$ and $3 \leq d(g_2) < \Delta$ holds. And by Theorem 13, we know that there is only one nonfull internal vertex in T^*. Then, it is easy to know that $W_1 \neq \varnothing, W_2 \neq \varnothing$ and $\min_{i \in W_2} d(i, \mathrm{and} r) \geq 2$ hold.

Suppose $\max_{i \in W_1} d(i, r) = m$, then $m = 1$. Assume that $m = 1$ is not established, then we have $m \geq 2$. Now choose a vertex u_1 which satisfies $d(u_1, r) = m$ and $u_1 \in W_1$ in T^*. Choose $u_2 \in N_{T^*}(u_1)$, then $x_{g_2} \leq x_{u_2}$. Otherwise, $x_{g_2} > x_{u_2}$, 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 $T_1 \in T_n^\Delta$. 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^Δ. Let $T_2 = T^* - (g_1, g_2) - (u_1, u_2) + (g_2, u_1) + (u_2, g_1)$, it is easy to know $T_2 \in T_n^\Delta$. From $x_{g_2} \leq x_{u_2}$, and by Lemma 10, we get $x_{g_1} > x_{u_1}$; 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_n^Δ. Hence, the hypothesis is not established, and then we have $m = 1$. From $\min_{i \in W_2} d(i, r) \geq 2$, we get $\max_{i \in W_2} d(i, r) \geq 2$. And for $\max_{i \in W_1} d(i, r) = 1$, by (3) of Theorem 17, we have that $\max_{i \in W_2} d(i, r) = 2$ holds. Thus, $\max_{i \in W_2} d(i, r) = \min_{i \in W_2} d(i, r) = 2$, from $\max_{i \in W_1} d(i, r) = 1$, and from 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 is $u_0 u_1 \cdots u_l \cdots u_k$, where $k > l$. From the definition of P_1, we know $u_l = w$, then we have that u_l 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_2 has no public edge with P_1, and the length of P_2 is $l + 2$. Suppose that P_2 is $u_0 v_1 \cdots v_{l+1} v_{l+2}$, 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_3 in which u_0 is the starting point and a leaf node of T^* is the terminal point. Besides, P_3 has no public edge with P_1, and from Theorem 17, we know that the length of P_3 is not less than $l + 1$. Hence, suppose that P_3 is $u_0 v_1 \cdots v_{l+1} \cdots$, and the relationship between P_1 and P_3 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

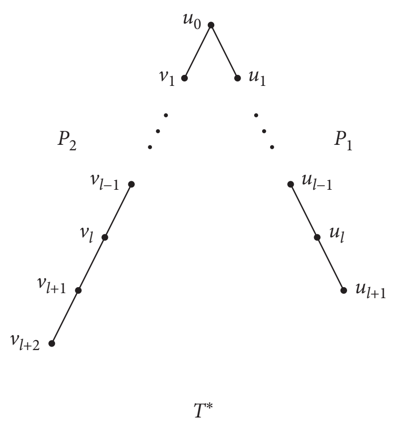

Figure 14: Vertex graphs of two paths under $k = l + 1$.

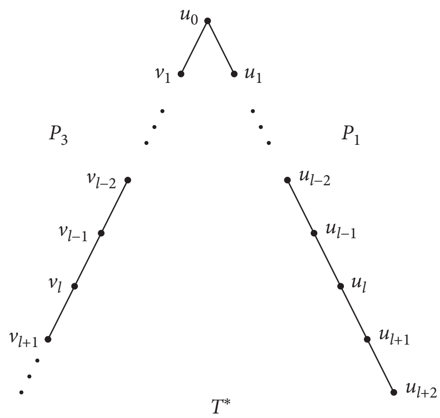

Figure 15: Vertex graphs of two paths under $k = l + 2$.

starting point and a leaf node of T^* is the terminal point. Besides, P_4 has no public edge with P_1, and from Theorem 17, we know that the length of P_4 is not less than $l + 2$. Hence, suppose that P_4 is $u_0 v_1 \cdots v_{l+2} \cdots$, and the relationship between P_1 and P_4 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 $x_{u_l} \geq x_{v_{l+1}}$, let $T_1 = T^* - (v_{l+2}, v_{l+1}) + (v_{l+2}, u_l)$, 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^{Δ}.

If $x_{u_l} < x_{v_{l+1}}$, and for $x_{u_0} = x_r \geq x_{v_1}$, we know that there exists a natural number k that satisfies $2 \leq k \leq l + 1$, which make that $x_{u_{k-1}} < x_{v_k}$ and $x_{u_{k-2}} \geq x_{v_{k-1}}$ hold. Let $T_2 = T^* - (v_{k-1}, v_k) - (u_{k-2}, u_{k-1}) + (v_k, u_{k-2}) + (u_{k-1}, v_{k-1})$, it is easy to know $T_2 \in T_n^{\Delta}$. From $x_{u_{k-1}} < x_{v_k}$ and $x_{u_{k-2}} \geq x_{v_{k-1}}$, and by Lemma 3, we have that $\rho(T_2) > \rho(T^*)$ holds, and this implies a

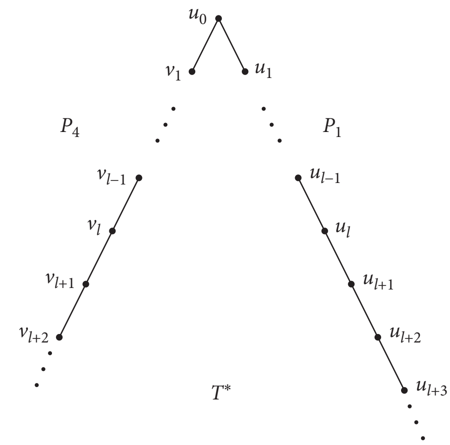

Figure 16: Vertex graphs of two paths under $k > l + 2$.

contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}.

Hence, subcase 1 of case 2 implies a contradiction.

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

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

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

If $x_{v_l} \geq x_{u_l}$, and for $x_{v_{l+1}} < x_{u_{l+1}}$, let $T_1 = T^* - (v_{l+1}, v_l) - (u_{l+1}, u_l) + (v_l, u_{l+1}) + (v_{l+1}, u_l)$, it is easy to know $T_1 \in T_n^{\Delta}$. 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^{Δ}; hence, $x_{v_l} < x_{u_l}$. Let $T_2 = T^* - (v_l, v_{l+1}) + (v_{l+1}, u_l)$, it is easy to know $T_2 \in T_n^{\Delta}$, 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^{Δ}.

Subcase 2.2. v_{l+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 $x_{v_i} \leq x_{u_l}$, then let $T_3 = T^* - (v_i, v_{i+1}) + (v_{i+1}, u_l)$, it is easy to know $T_3 \in T_n^{\Delta}$. 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^{Δ}. Hence, for arbitrary vertex v_i which satisfies $1 \leq i \leq l + 1$, we all have $x_{v_i} > x_{u_l}$. Specially, we have $x_{v_{l+1}} > x_{u_l}$.

From $x_{u_0} \geq x_{v_1}$ and $x_{v_{l+1}} > x_{u_l}$, we know that there exists a natural number k that satisfies $2 \leq k \leq l + 1$, which makes both $x_{v_k} > x_{u_{k-1}}$ and $x_{v_{k-1}} \leq x_{u_{k-2}}$ hold. Let $T_4 = T^* - (v_k, v_{k-1}) - (u_{k-1}, u_{k-2}) + (v_k, u_{k-2}) + (u_{k-1}, v_{k-1})$, it is easy to know $T_4 \in T_n^{\Delta}$. From $x_{v_k} > x_{u_{k-1}}$ and $x_{v_{k-1}} \leq x_{u_{k-2}}$, 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^{Δ}.

Hence, in subcase 2, no matter whether v_{l+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. Then, 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_n^{Δ}, $T^* \not\cong T_{n,2}^{\Delta}$ 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_n^{Δ}, $x = (x_1, x_2, \ldots, x_n)^T$ 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 $W_1 = \{i|i$ is the leaf node of T^*, and the shortest path from i to r neither pass g_1 nor pass $g_2\}$, $W_2 = \{i|i$ is the leaf node of T^*, and the shortest path from i to r either pass g_1 or pass $g_2\}$. Assume that $T^* \not\cong T_{n,2}^{\Delta}$, that is $W_2 \neq \varnothing$, 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 $j_1 \in W_2$ which makes (u, j_1) is a pendant edge or $u \in V(C)$ and $d(u) = 2$.

(3) If $\max_{i\in W_1} d(i, r) \neq \min_{i\in W_1} d(i, r)$, then there exists a leaf node $j_1 \in W_1$ which makes (u, j_1) is a pendant edge.

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 $W_2 \neq \varnothing$, we know $\max_{i\in W_2} d(i, r) \geq 2$; 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 $W_2 \neq \varnothing$, 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, $\max_{i\in W_1} d(i, r) = 1$. 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 $u_1 \in W_2$ such that (u_1, u) is a pendant edge of T^*. Let $u_1 u_2 \cdots u_m r$ be the shortest path from u_1 to r, where $u_2 = u$, $u_m = g_1$, 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 $\forall j_1 \in W_1$, we all have $d(j_1, r) = 2$. 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 $x_{g_2} > x_{v_1}$ holds. From $u_m = g_1$ and $m = 2$, we get $g_1 = u_2$, and by $u_2 = u$, we have $u_m = u = g_1$. In addition, for the relationship of x_{g_1} and x_{v_2}, we must have $x_{g_1} \leq x_{v_2}$. 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 $T_1 \in T_n^{\Delta}$. 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^{Δ}. 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 $T_2 \in T_n^{\Delta}$. From $x_{g_2} > x_{v_1}$ and $x_{g_1} \leq x_{v_2}$, 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^{Δ}. 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 since $d(u_1, r) = m$, where $u_1 \in W_2$, then for $\forall j_1 \in W_1$, we all have that $d(j_1, r) = m$ holds. Choose $j_1 \in W_1$, then we have that $d(j_1, r) = m$ holds. Without loss of generality, we assume that the shortest path from j_1 to r is $v_1 v_2 \cdots v_m r$, where $v_1 = j_1$, $v_m \neq g_1$ and $v_m \neq g_2$.

Since $u_2 = u$ is the nonfull internal vertex, then we have $x_{u_2} < x_{v_2}$. Otherwise, $x_{u_2} \geq x_{v_2}$, let $T_3 = T^* - (v_1, v_2) + (v_1, u_2)$, and it is easy to know $T_3 \in T_n^{\Delta}$. 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^{Δ}. Hence, $x_{u_2} < x_{v_2}$.

For $m \geq 3$, hence u_3 and v_3 have the meaning. For the relationship between x_{u_3} and x_{v_3}, we have that $x_{u_3} < x_{v_3}$ holds. Otherwise, $x_{u_3} \geq x_{v_3}$, let $T_4 = T^* - (u_3, u_2) - (v_3, v_2) + (v_3, u_2) + (v_2, u_3)$, and it is easy to know $T_4 \in T_n^{\Delta}$. Since $x_{u_3} \geq x_{v_3}$ and $x_{u_2} < x_{v_2}$, 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_n^{Δ}. 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 $x_{u_2} > x_{v_1}$. For the relationship between x_{u_3} and x_{v_2}, we have $x_{u_3} > x_{v_2}$. Otherwise, $x_{u_3} \leq x_{v_2}$, let $T_5 = T^* - (u_3, u_2) - (v_1, v_2) + (v_1, u_3) + (v_2, u_2)$, and it is easy to know $T_5 \in T_n^{\Delta}$. From $x_{u_2} > x_{v_1}$ and $x_{u_3} \leq x_{v_2}$, 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^{Δ}. 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 $x_{v_m} > x_{u_m} > x_{v_{m-1}}$.

For the relationship between x_{g_2} and x_{v_m}, we have $x_{g_2} > x_{v_m}$. Otherwise, $x_{g_2} \leq x_{v_m}$. Let $T_6 = T^* - (u_m, g_2) - (v_{m-1}, v_m) + (g_2, v_{m-1}) + (v_m, u_m)$, and it is easy to know $T_6 \in T_n^{\Delta}$. From $x_{g_2} \leq x_{v_m}$ and $x_{u_m} > x_{v_{m-1}}$, 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^{Δ}.

Thus, we have that $x_{g_2} > x_{v_m} > x_{u_m} > x_{v_{m-1}}$ 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 $T_7 \in T_n^{\Delta}$. 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^{Δ}.

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

(2) Assume that (2) of Theorem 19 does not hold, then the nonfull internal vertex u in T^* should satisfy that there exists $v_1 \in W_1$ such that (v_1, u) is a pedant edge. For there exist two leaf nodes i, j in T^* such that $d(i, r) \neq d(j, r)$ and $\max_{i \in W_1} d(i, r) = \min_{i \in W_1} d(i, r)$. Hence by Theorem 17, we know $\max_{j_2 \in W_2} d(j_2, r) = \max_{j_1 \in W_1} d(j_1, r) + 1$; 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.

(3) Since $W_2 \neq \varnothing$ and $\max_{i \in W_1} d(i, r) \neq \min_{i \in W_1} d(i, r)$, by Theorem 17, we get $\max_{i \in W_2} d(i, r) = \min_{i \in W_2} d(i, r) = \max_{i \in W_1} d(i, r) = \min_{i \in W_1} d(i, r) + 1$. And it is easy to know $\min_{i \in W_1} d(i, r) \geq 1$; hence, $\max_{i \in W_1} d(i, r) \geq 2$. 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 $j_1 \in W_2$ such that (j_1, u) is a pedant edge of T^*. From $W_2 \neq \varnothing, d(g_1) \geq 3$, and $d(g_2) \geq 3$, we have that $d(j_1, r) \geq 2$ holds.

Now we will prove $d(j_1, r) \geq 3$. Assume that $d(j_1, r) \geq 3$ does not hold, then we have $d(j_1, r) = 2$, by $\max_{i \in W_2} d(i, r) = \min_{i \in W_2} d(i, r) = \max_{i \in W_1} d(i, r) = \min_{i \in W_1} d(i, r) + 1$, we know that there exists $i \in W_1$ such that $d(i, r) = 2$. Let the shortest path from i to r be $v_1 v_2 r$, where $v_1 = i, v_2 \neq g_1$, and $v_2 \neq g_2$, and let the shortest path from j_1 to r be $u_1 u_2 r$, where $j_1 = u_1, u_2 = u$, and u_2 is either g_1 or g_2. Without loss of generality, we assume that $u_2 = g_1$, and it is easy to know $x_{v_2} > x_{u_2}$; otherwise, $x_{v_2} \leq x_{u_2}$. Let $T_1 = T^* - (v_1, v_2) + (u_2, v_1)$, then it is easy to know $T_1 \in T_n^{\Delta}$, and by Lemma 1, we have that $\rho(T_1) > \rho(T^*)$ holds. This implies a contradiction with T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}; hence, $x_{v_2} > x_{u_2}$. For $u_2 = g_1$, thus, we get $x_{v_2} > x_{g_1}$. And for v_1 is the leaf node of T^*, g_2 is the nonleaf node of T^*, and then by Lemma 10, we have $x_{g_2} > x_{v_1}$. Thus, we get that $x_{v_2} > x_{g_1}$ and $x_{g_2} > x_{v_1}$ hold. Let $T_2 = T^* - (v_1, v_2) - (g_1, g_2) + (v_2, g_2) + (g_1, v_1)$, 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^{Δ}. Thus, the hypothesis does not hold; hence, $d(j_1, r) \geq 3$.

Suppose that the shortest path from j_1 to r is $u_1 u_2 \cdots u_{m+1} r$, where $u_1 = j_1$, $u_2 = u$, and $u_{m+1} = g_1$ or $u_{m+1} = g_2$. Without loss of generality, we assume that $u_{m+1} = g_1$. From $d(j_1, r) \geq 3$, we can get $m \geq 2$. Since $\max_{i \in W_2} d(i, r) = \min_{i \in W_2} d(i, r) = \max_{i \in W_1} d(i, r) = \min_{i \in W_1} d(i, r) + 1$, there exists $i \in W_1$ such that $d(i, r) = d(j_1, r)$.

Suppose that the shortest path from i to r is $v_1 v_2 \cdots v_{m+1} r$, where $v_1 = i, v_{m+1} \neq g_1$, and $v_{m+1} \neq g_2$. For the relationship between x_{v_2} and x_{u_2}, we have $x_{v_2} > x_{u_2}$. Otherwise, $x_{v_2} \leq x_{u_2}$. Let $T_3 = T^* - (v_1, v_2) + (u_2, v_1)$, then it is easy to know $T_3 \in T_n^{\Delta}$. And 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^{Δ}. In addition, we also can prove $x_{v_3} > x_{u_3}$; otherwise, $x_{v_3} \leq x_{u_3}$. Let $T_4 = T^* - (u_2, u_3) - (v_2, v_3) + (u_2, v_3) + (v_2, u_3)$, then it is easy to know $T_4 \in T_n^{\Delta}$. From $x_{v_2} > x_{u_2}$ and $x_{v_3} \leq x_{u_3}$, 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^{Δ}; hence, $x_{v_3} > x_{u_3}$. By mathematics induction, we can prove that, for any natural number i which satisfies $2 \leq i \leq m + 1$, we all have that $x_{v_i} > x_{u_i}$ holds.

By Lemma 10, we can get $x_{u_2} > x_{v_1}$. For the relationship between x_{u_3} and x_{v_2}, we have $x_{u_3} > x_{v_2}$. Otherwise, $x_{u_3} \leq x_{v_2}$. Let $T_5 = T^* - (u_3, u_2) - (v_1, v_2) + (v_1, u_3) + (v_2, u_2)$, then it is easy to know $T_5 \in T_n^{\Delta}$. From $x_{u_2} > x_{v_1}$ and $x_{u_3} \leq x_{v_2}$, 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^{Δ}. 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 $x_{v_{m+1}} > x_{u_{m+1}} > x_{v_m}$.

Besides, for the relationship between x_{g_2} and $x_{v_{m+1}}$, we have $x_{g_2} > x_{v_{m+1}}$. Otherwise, $x_{g_2} \le x_{v_{m+1}}$. Let $T_6 = T^* - (g_1, g_2) - (v_m, \quad v_{m+1}) + (g_1, v_{m+1}) + (g_2, v_m)$, then it is easy to know $T_6 \in T_n^{\Delta}$. By $g_1 = u_{m+1}$ and $x_{u_{m+1}} > x_{v_m}$, we can get $x_{g_1} > x_{v_m}$. And for $x_{g_2} \le x_{v_{m+1}}$, 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^{Δ}. Let $T_7 = T^* - (g_2, u_{m+1}) - (v_m, v_{m+1}) + (g_2, v_{m+1}) + (u_{m+1}, v_m)$, then it is easy to know $T_7 \in T_n^{\Delta}$. From $x_{g_2} > x_{v_{m+1}}$ and $x_{v_{m+1}} > x_{u_{m+1}} > x_{v_m}$, we can get $x_{g_2} > x_{v_{m+1}} > x_{u_{m+1}} > x_{v_m}$. 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^{Δ}.

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 the number of vertices and the maximum degree; in the following Theorem, we describe the structure of the maximal-adjacency-spectrum unicyclic graphs in T_n^{Δ}. □

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^{Δ} if and only if $T^* \cong H_n^{\Delta}$.*

Proof. Necessity, suppose that $T^* \in T_n^{\Delta}$, T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}, let $x = (x_1, x_2, \ldots, x_n)$ 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, $T^* \cong H_n^{\Delta}$.

When the level of T^* is 3, if there is no nonfull internal vertex in C, then it is easy to know that $T^* \cong H_n^{\Delta}$ 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, $W_2 = \varnothing$. From (1) of Theorem 17, we know $T^* \cong T_{n,2}^{\Delta}$, 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, $T^* \cong H_n^{\Delta}$.

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 $V(C) = \{r, g_1, g_2\}$; we have $\max_{j \in W_2} d(j, r) = \min_{j \in W_2} d(j, r) = 2$. Then, by (4) of Theorem 17, we get $\max_{j \in W_1} d(j, r) \le 2$.

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 $r u_2 u_1$, where $u_1 = i$, and u_2 is neither g_1 nor g_2. According to the relationship between x_{g_2} and x_{u_2}, we have $x_{g_2} < x_{u_2}$. Otherwise, $x_{g_2} \ge x_{u_2}$, 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^{Δ}. 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 $x_{g_1} > x_{u_1}$. And we have proved $x_{g_2} < x_{u_2}$; 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^{Δ}; hence, $\max_{j \in W_1} d(j, r) = 1$. From that $\max_{j \in W_2} d(j, r) = \min_{j \in W_2} d(j, r) = 2, \max_{j \in W_1} d(j, r) = 1$ and there is only one nonfull internal vertex in C, we know that $T^* \cong H_n^{\Delta}$ holds.

In conclusion, when the level of T^* is 3, we have that $T^* \cong H_n^{\Delta}$ 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 $k \ge 3$.

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 $g_2\}$, $Q_2 = \{i \in V(T^*) | d(i, r) = k - 1$, 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 $V(T^*) \backslash V(C)$. 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 $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r)$.

At this time, from Theorem 17, we get $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i, r) = \max_{i\in W_2} d(i,r) - 1 = k-1$. And for $\forall q_1 \in Q_1$, we all have that $d(q_1) = 1$ holds.

Subcase 3. When $\max_{i\in W_1} d(i,r) \neq \min_{i\in W_1} d(i,r)$.

At this time, from Theorems 17 and 19, we know that the following two conclusions hold. ① $\max_{i\in W_2} d(i,r) = \min_{i\in W_2} d(i, r) = \max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r) + 1$. ② $\forall q_2 \in Q_2$ 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 $d(i,r) \neq d(j,r)$ and $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r)$.

At this time, from Theorems 17 and 19, we know that the following three conclusions hold: ① $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r) = \max_{i\in W_2} d(i,r) - 1 = k-1$; ② $\forall q_1 \in Q_1$ all have that $d(q_1) = 1$ holds; ③ the nonfull internal vertex $u \in Q_2$.

Subcase 2. When $\max_{i\in W_1} d(i,r) \neq \min_{i\in W_1} d(i,r)$.

From Theorems 17 and 19, we know that the following three conclusions hold: ① $\max_{i\in W_2} d(i,r) = \min_{i\in W_2} d(i,r) = \max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r) + 1$. ② $\forall q_2 \in Q_2$ all have that $d(q_2) = \Delta$ holds. ③ The nonfull internal vertex $u \in Q_1$.

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 $u \in Q_1$, and $\forall q_2 \in Q_2$ all have that $d(q_2) = \Delta$ holds. And for there is only one nonfull internal vertex in T^*, then we have that, for $\forall j_1 \in Q_1 \backslash \{u\}$, we all have $d(j_1) = \Delta$; hence, $T^* \cong H_n^{\Delta}$ holds.

Subcase 2. When there two exist leaf nodes i, j in T^*, which make $d(i,r) \neq d(j,r)$ and $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r)$.

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 $d(i,r) \neq d(j,r)$ and $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r)$ in T^*, by Theorem 17, we get $\max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r) = k-1$.

Subcase 3. When $\max_{i\in W_1}(d(i,r)) \neq \min_{i\in W_1}(d(i,r))$.

At this time, from Theorem 19, we get $u \in Q_1$. Since $\max_{i\in W_1}(d(i,r)) \neq \min_{i\in W_1}(d(i,r))$, by (3) and (4) of Theorem 17, we can get $\max_{i\in W_2} d(i,r) = \min_{i\in W_2} d(i,r) = \max_{i\in W_1} d(i,r) = \min_{i\in W_1} d(i,r) + 1$. And for there is only one nonfull internal vertex u in T^*, and $u \in Q_1$; hence, for $\forall q_2 \in Q_2$, we all have $d(q_2) = \Delta$.

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 $\max_{i\in W_1 \cup W_2} d(i,r) = k$ $(k \geq 3)$, 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: ① except r, g_1, g_2, if $w_i \in V(T^*)$, then let w_i express one of the vertices in the bottom layer of the first i of T^*. ② If $w_i \in V(T^*)$, we denote w_j $(j > i)$ the ancestor of w_i, which is in the bottom layer of the first j of T^*, (note: w_i 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 ① and ② are still established when w is changed for any other vertex, which is not g).

Assume that $T^* \ncong H_n^{\Delta}$, 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 $r_2 = u$), which make u, s_2 satisfy the following properties: ① s_2 at least has one full-degree brother. ② The common direct ancestor of s_2 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_l $(l \geq 4)$, 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 $T_1 \in T_n^{\Delta}$. 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^{Δ}; 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 $T_2 \in T_n^{\Delta}$. If $x_{r_3} \leq x_{s_3}$, 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^{Δ}; hence, $x_{r_3} > x_{s_3}$. Let $T_3 = T^* - (v_2, s_3) - (r_2, r_3) + (r_2, s_3) +$

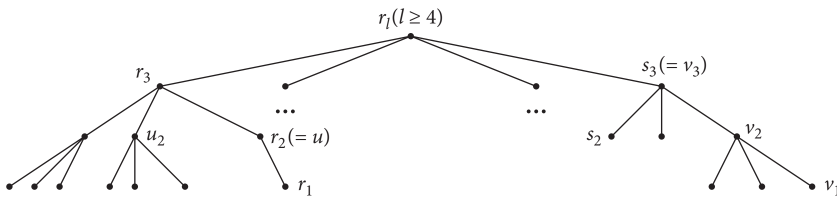

Figure 17: Vertex graph in case 1.

(v_2, r_3), then it is easy to know that $T_3 \in T_n^{\Delta}$. From $x_{r_2} < x_{v_2}$ and $x_{r_3} > x_{s_3}$, 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^{Δ}. Hence, the hypothesis is not established; therefore, $T^* \cong H_n^{\Delta}$.

Case 4. For T^* is an almost full-degree unicyclic graph with root node r, $T^* \ncong H_n^{\Delta}$, 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_2 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, andv_2 of the nearest generation, and u_2 and v_2 satisfy that $u_2 \neq v_2, r_t \neq w$, $s_m \neq w$ 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 $\max\{x_{r_2}, x_{s_2}\} < \min\{x_{u_2}, x_{v_2}\}$.

If $x_{u_t} \geq x_{s_t}$, then $x_{r_t} \geq x_{v_t}$. Since $x_{r_2} < x_{v_2}$, there is a natural number k that satisfies $2 \leq k \leq t-1$, which make $x_{r_k} < x_{v_k}$ and $x_{r_{k+1}} \geq x_{v_{k+1}}$. Let $T_1 = T^* - (r_{k+1}, r_k) - (v_{k+1}, v_k) + (r_{k+1}, v_k) + (v_{k+1}, r_k)$, then it is easy to know $T_1 \in T_n^{\Delta}$. From $x_{r_k} < x_{v_k}$ and $x_{r_{k+1}} \geq x_{v_{k+1}}$, 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^{Δ}.

If $x_{u_t} < x_{s_t}$, since $x_{u_2} > x_{s_2}$, there exists a natural number k that satisfies $2 \leq k \leq t-1$, which makes $x_{u_k} > x_{s_k}$ and $x_{u_{k+1}} \leq x_{s_{k+1}}$. Let $T_2 = T^* - (u_{k+1}, u_k) - (s_{k+1}, s_k) + (u_{k+1}, s_k) + (s_{k+1}, u_k)$, then it is easy to know $T_2 \in T_n^{\Delta}$. From $x_{u_k} > x_{s_k}$ and $x_{u_{k+1}} \leq x_{s_{k+1}}$, 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^{Δ}.

Hence, the hypothesis is not established; therefore, $T^* \cong H_n^{\Delta}$.

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

By considering the discussion of all the cases according to the level of T^*, we know that if $T^* \in T_n^{\Delta}$, 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^{Δ}, then $T^* \cong H_n^{\Delta}$.

Sufficiency, suppose that $T^* \in T_n^{\Delta}$, 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 $T^* \cong H_n^{\Delta}$. It is easy to know $|T_n^{\Delta}| < +\infty$, then there must exist maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}. Suppose that T^{**} is a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}, 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 $T^{**} \cong H_n^{\Delta}$. And for $T^* \cong H_n^{\Delta}$, then $T^{**} \cong T^*$; thus, T^* is a maximal-adjacency-spectrum unicyclic graph in T_n^{Δ}.

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

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
$K(T) = \max_{1 \leq i \leq r}\{\max\{d(v_i, u) \cdot u \in V(B_i)\}\} + 1$.

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 $\Delta \geq 4$, then we have $\rho(T) < 2\sqrt{\Delta - 1}\cos(\pi/(2K(T) + 1))$.*

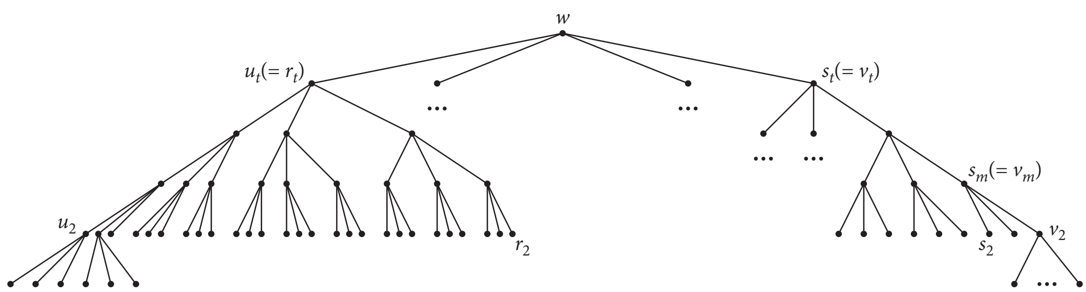

FIGURE 18: Vertex graph in case 2.

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 Δ, which satisfy $n > \Delta \geq 3$. We suppose that F_1 is a unicyclic graph with the maximum degree Δ, 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 Δ.

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 $W_1(F_1) = \{i|i$ is the leaf node of F_1, and the shortest path from i to r neither pass g_1 nor pass $g_2\}$, $W_2(F_1) = \{i|i$ 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 $\min_{i\in W_1(F_1)} d(i,r) + 1 = \max_{i\in W_1(F_1)} d(i,r) + 1 = \min_{i\in W_2(F_1)} d(i,r) = \max_{i\in W_2(F_1)} d(i,r)$ hold.

Then, we call F_1 is a completely Bethe unicyclic graph with the maximum degree Δ, 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 Δ, which satisfy $n > \Delta \geq 3$. Let F be a completely Bethe unicyclic graph with the maximum degree Δ, 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 Δ, 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 Δ, 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 Δ, the length of the circle is 3, and the adjacency spectral radius is not less than $\rho(H_n^{\Delta})$ by $F_{n,\Delta}^*$.

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

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

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

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

$$A_a = \begin{bmatrix} 0 & \sqrt{\Delta-1} & 0 & \cdots & \cdots & 0 \\ \sqrt{\Delta-1} & 0 & 0 & \ddots & & \vdots \\ 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \sqrt{\Delta-1} & 0 \\ \vdots & & \ddots & \sqrt{\Delta-1} & 0 & \sqrt{\Delta-2} \\ 0 & \cdots & \cdots & 0 & \sqrt{\Delta-2} & 2 \end{bmatrix}_{a\times a},$$

then we have that $\rho(B_{m(n,\Delta)}^{a}) = \rho(A_a)$ 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 $\rho(B_{m(n,\Delta)}^{a}) < 2\sqrt{\Delta-1}\cos(\pi/(2a+1))$ holds.*

Proof. By the definition of $B_{m(n,\Delta)}^{a}$ 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 $T \cong B_6^2$, that is $T \cong H_6^3$.

(2) When $\Delta = 3$ and $7 < n \leq 12$, we have that $\rho(T) \leq \rho_1$ holds, where ρ_1 is the maximum real root of the

equation $\lambda^3 - 2\lambda^2 - 3\lambda + 2 = 0$, and the necessary and sufficient condition for the equal sign is $T \cong B_{12}^3$, that is, $T \cong H_{12}^3$. Through the calculation by Matlab, we get $\rho_1 = 2.5616$.

(3) *When $\Delta = 3$ and $n \geq 13$, or when $\Delta \geq 4$, we all have that $\rho(T) < 2\sqrt{\Delta - 1}\cos(\pi/(2a+1))$ holds, where $a = \lceil \log_{\Delta-1}(n/3) \rceil + 1$.*

Proof. (1) When $\Delta = 3$ and $n \leq 6$, it is easy to know $F_{n,\Delta}^* = B_6^2$; by the definition of B_6^2 and Theorem 20, it is easy to have that $\rho(T) \leq \rho(B_6^2)$ holds. From Theorem 20, we know that the equal sign establishes if and only if $T \cong B_6^2$. If we denote $A_2 = \begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix}$, then from Lemma 11, we know that $\rho(B_6^2) = \rho(A_2)$ 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 $T \cong B_6^2$, that is, $T \cong H_6^3$.

(2) When $\Delta = 3$ and $7 < n \leq 12$, it is easy to know $F_{n,\Delta}^* = B_{12}^3$; 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 $T \cong B_{12}^3$. 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 ρ_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 $T \cong B_{12}^3$, that is, $T \cong H_{12}^3$.

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

4.2. The Comparison of the Results in Theorems 21 and 22. Choose $T \in T_{19}^4$, where T is shown in Figure 19. By Lemma 11, we have that $\rho(T) < 2\sqrt{3}\cos(\pi/15)$ holds, and by Theorem 22, we get $\rho(T) < 2\sqrt{3}\cos(\pi/7)$. Obviously, we have that $2\sqrt{3}\cos(\pi/7) < 2\sqrt{3}\cos(\pi/15)$ holds; that is, the upper bound of $\rho(T)$ that Theorem 22 gives is better than the one that Theorem 21 gives.

Actually, when $T \in T_n^\Delta$ 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.

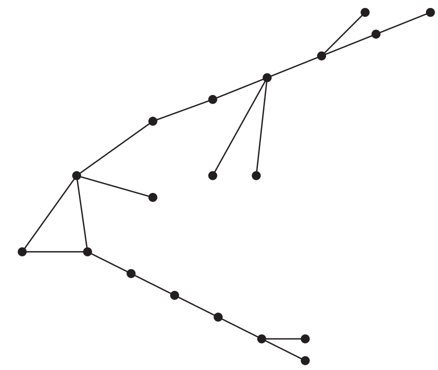

Figure 19: A unicyclic graph with maximum degree 4 and vertex number 19.

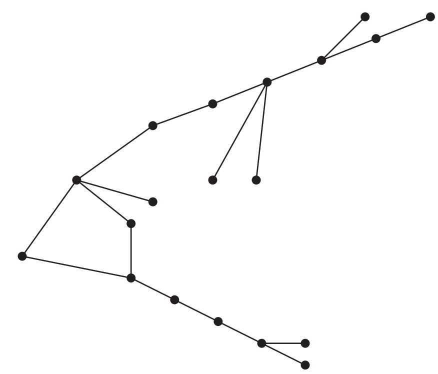

Figure 20: Another unicyclic graph with maximum degree 4 and vertex number 19.

Choose $T_1 \in T_{19}^4$, where T_1 is shown in Figure 20. By Theorem 21, we have that $\rho(T_1) < 2\sqrt{3}\cos(\pi/15)$ holds, and by Theorem 22, we can get $\rho(T_1) < 2\sqrt{3}\cos(\pi/7)$. Obviously, we have that $2\sqrt{3}\cos(\pi/7) < 2\sqrt{3}\cos(\pi/15)$ 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 $T \in T_n^\Delta$ 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.

Acknowledgments

This research was supported by the Scientific Research Foundation of Huaqiao University (10HZR26) and the Natural Science Foundation of Fujian Province (Z0511028).

References

[1] H. Sachs, "Beziehungen zwischen den in einem graphen enthaltenen kreisen und seinem cgarakteristischen polynom," *Publicationes Mathematicae Debrecen*, vol. 11, pp. 119–134, 1964.

[2] L. Collatz and U. Sinogowitz, "Spektren endlicher grafen," *Abhandlungen aus dem Mathematischen Seminar der Universität Hamburg*, vol. 21, pp. 63–77, 1957.

[3] S. Hu, "The largest eigenvalue of unicyclic graph," *Discrete Mathematics*, vol. 307, pp. 280–284, 2007.

[4] A. J. Hoffman, "The change in the least eigenvalue of the adjacent matrix of a graph under imbedding," *SIAM Journal on Applied Mathematics*, vol. 17, pp. 664–677, 1969.

[5] R. Merris, "Laplacian matrices of graphs: a survey," *Linear Algebra and Its Applications*, vol. 197-198, pp. 143–176, 1994.

[6] M. Fisher, "On hearing the shape of a drum," *Journal of Combinatorial Theory*, vol. 1, pp. 105–125, 1966.

[7] S. G. Guo, G. H. Xu, and Y. G. Chen, "On the spectral radius of trees with n vertices and diameter d," *Advances in Mathematics (China)*, vol. 34, no. 6, pp. 683–692, 2005, in Chinese.

[8] S. G. Guo and J. Y. Shao, "On the spectral radius of trees with fixed diameter," *Linear Algebra and Its Applications*, vol. 413, no. 1, pp. 131–147, 2006.

[9] M. Petrovic, I. Gutman, and S. G. Guo, "On the spectral radius of bicyclic graph," *Bulletin: Classe des Sciences Mathematiques et Natturalles*, vol. 22, no. 4, pp. 93–99, 2005.

[10] S. G. Guo, "The spectral radius of unicyclic and byicyclic graph with n vertices and k pendent vertices," *Linear Algebra and Its Applications*, vol. 408, pp. 78–85.

[11] S. G. Guo, "On the spectral radius of bycyclic graph with n vertices and diameter d," *Linear Algebra and Its Applications*, vol. 422, pp. 119–132, 2007.

[12] H. Q. Liu, M. Lu, and F. Tian, "On the spectral radius of unicyclic graph with n vertices and diameter d," *Linear Algebra and Its Applications*, vol. 420, pp. 449–459, 2007.

[13] F. Belardo, E. M. L. Marzi, S. K. Simić, and J. F. Wang, "On the spectral radius of unicyclic graph with prescribed degree sequence," *Linear Algebra and Its Applications*, vol. 432, pp. 2323–2334, 2010.

[14] D. M. Cvetkovic and P. Rowlinson, "The largest eigenvalues of graph," *Linear Multilinear Algebra*, vol. 28, pp. 3–33, 1990.

[15] O. Rojo, "The spectra of a graph obtained from copies of a generalized Bethe tree," *Linear Algebra and Its Applications*, vol. 420, no. 2-3, pp. 490–507, 2007.

[16] O. Rojo, "New upper bounds on the spectral radius of unicyclic graph," *Linear Algebra and Its Applications*, vol. 428, pp. 754–764, 2008.