Ordering graphs with maximum degree 3 by their indices *

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Abstract We consider the connected graphs with a unique vertex of maximum degree 3. Two subfamilies of such graphs are characterized and ordered completely by their indices. Moreover, a conjecture about the complete ordering of all graphs in this set is proposed.

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1 Introduction

In this paper we only consider finite simple graphs (without loops or multiple edges). The spectrum of a graph G is the spectrum of $A(G)$, the adjacent matrix of the graph G. The largest eigenvalue of $A(G)$ is called the index (or spectral radius) of G, and is denoted by $\rho(G)$. The characteristic polynomial of G is just $det(xI - A(G))$, which is denoted by $\Phi(G, x)$, or simply by $\Phi(G)$. For other undefined notions and terminology on the algebraic graph theory, the readers are referred to [1].

To classify and order graphs by their indices is an interesting problem proposed by Cvetković in [2]. In [3], Smith determined all the graphs with index not exceed 2. In [4] Cvetković et al. listed the graphs with index in the interval $(2, \sqrt{2+\sqrt{5}})$, all of which are trees. Recently many authors

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studied the ordering of some special families of graphs, such as trees, see [5], etc.

In this paper, we focus on the connected graphs with a unique vertex of maximum degree 3. Let $U_n(3)$ be the set of connected graphs on n vertices and having a unique vertex of maximum degree 3. In Section 2, we give some lemmas which will be used in the proofs. In Section 3, two subsets of graphs of $U_n(3)$ are characterized and completely ordered, also a conjecture is posed about the complete ordering of $U_n(3)$.

2 Some lemmas

Before proving our main results, we first give the following six lemmas as some necessary preliminaries.

Lemma 2.1 ([6]). *Let $G(m,n)$ be a graph obtained from a non-trivial connected graph G by attaching at some fixed vertex two pendant paths whose lengths are m and n, respectively. If $m \geq n \geq 1$, then $\rho(G(m,n)) > \rho(G(m-1,n+1))$.*

For positive integers a, b and c, we denote by $T(a,b,c)$ a tree such that for some vertex $v \in V(T(a,b,c))$, $T(a,b,c) - v = P_a \bigcup P_b \bigcup P_c$.

Lemma 2.2 ([7]). *Let v_q be the largest real root of the polynomial*

$$L_q(v) = v^q - (v^{q-2} + v^{q-3} + \cdots + v + 1).$$

We set $\lambda_q = v_q^{\frac{1}{2}} + v_q^{-\frac{1}{2}}$, and $\lambda_\infty = v_\infty^{\frac{1}{2}} + v_\infty^{-\frac{1}{2}}$. Then $2 = \lambda_2 < \lambda_3 < \cdots \lambda_q < \lambda_{q+1} < \cdots < \lambda_\infty = \sqrt{2+\sqrt{5}} \approx 2.058171$. Moreover, $\rho(T(2,2,c))$ increases strictly with c and converges to λ_∞.

Remark 2.1. *It is pointed out in [1] that if G is a connected graph, which is neither a tree nor a cycle, then $\rho(G) > \tau^{\frac{1}{2}} + \tau^{-\frac{1}{2}} = \sqrt{2+\sqrt{5}}$ where $\tau = \frac{\sqrt{5}+1}{2}$.*

Lemma 2.3 ([3]). *The only connected graphs on n vertices with index smaller than 2 are the path P_n, the graph Z_n and T_1, T_2 and T_3(see Fig. 1); The only connected graphs on n vertices with index equal to 2 are the cycle C_n, the graph W_n, and T_4, T_5 and T_6 (see Fig. 2).*

A path $P = v_0, v_1, \cdots, v_k$ is defined (see [8]) to be *an internal path* if one of the following holds:

(i) $k \geq 2$, $v_0, v_1, \cdots, v_k$ are all distinct, $d(v_0) \geq 3$, $v_0v_k \in E(G)$, and $d(v_i) = 2$, for all $i \in \{1, 2, \cdots, k\}$;

(ii) $k \geq 1$, $d(v_0) \geq 3$,$d(v_k) \geq 3$, and $d(v_i) = 2$, for all $i \in \{1, 2, \cdots, k-1\}$.

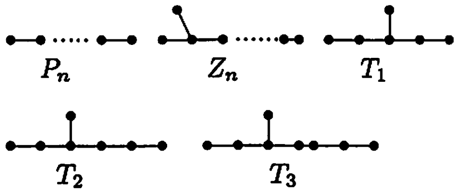

Fig. 1 The graphs with index smaller than 2

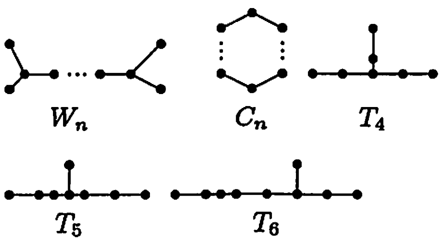

Fig. 2 The graphs with index equal to 2

Lemma 2.4 ([8]). *Let G be a connected graph and let G_{uv} be a graph obtained from G by subdividing the edge uv of G. If uv lies on an internal path of G, and $G \neq W_n$(see Fig.2), then $\rho(G_{uv}) < \rho(G)$.*

Let $x = 2cos\theta$, set $t^{\frac{1}{2}} = e^{i\theta}$, it is useful to write the characteristic polynomial of P_n, C_n in the following form(see [9]):

$$\Phi(P_n, t^{\frac{1}{2}} + t^{-\frac{1}{2}})) = t^{-\frac{n}{2}}(t^{n+1} - 1)/(t-1), \quad (1)$$

$$\Phi(C_n, t^{\frac{1}{2}} + t^{-\frac{1}{2}})) = t^{\frac{n}{2}} + t^{-\frac{n}{2}} - 2. \quad (2)$$

The following equation from [9] holds:

$$\Phi(T(a,b,c), t^{\frac{1}{2}} + t^{-\frac{1}{2}})t^{(a+b+c+1)/2}(t-1)^3 = t^{a+b+c+4} - 2t^{a+b+c+3} + t^{b+c+2} + t^{a+c+2} + t^{a+b+2} - t^{c+2} - t^{b+2} - t^{a+2} + 2t - 1. \quad (3)$$

Lemma 2.5 ([10]). *Let G be a graph. Denote by $\theta(e)$ the set of all cycles in G containing an edge $e = uv$, then we have: $\Phi(G,x) = \Phi(G-e,x) - \Phi(G-u-v,x) - 2\sum_{C\in\theta(e)}\Phi(G-V(C),x)$.*

Lemma 2.6 ([1]). *The increase of any element of a non-negative matrix A does not decrease the largest eigenvalue of A. The greatest eigenvalue increase strictly if A is an irreducible matrix. Therefore, in a connected graph G whose edge are assigned non-negative weights, every proper subgraph has smaller index than G.*

3 Main results

Now we only consider the graphs with a unique vertex of maximum degree 3, i.e. the ones of in $U_n(3)$. We denote by $C_k^{(l)}$ the graph obtained from a cycle C_k by attaching at one vertex of C_k a pendant path of length l. By the following theorem, the set $U_n(3)$ is totally divided into two subsets of graphs.

Theorem 3.1. *For any graph G, $G \in U_n(3)$ if and only if G is either a tree $T(a,b,c)$ for some integers a, b and c, or a unicyclic graph $C_k^{(l)}$ for some k and l.*

Proof. Both $T(a,b,c)$ and $C_k^{(l)}$ are obviously in the set $U_n(3)$.

Suppose that $G \in U_n(3)$. If G is a tree, from the definition of $U_n(3)$, G must be a tree $T(a,b,c)$ for some a, b and c. Otherwise, assume that G contains a cycle. If G contains two cycles C_p and C_q. Then one of the following three cases occurs:

(i) C_p and C_q share one vertex;

(ii) C_p and C_q share at least one edge;

(iii) C_p and C_q are linked by a path.

Any case will contradicts to the uniqueness of maximum degree 3. So G contains only one cycle, that is, G must be a $C_k^{(l)}$ for some k and l. □

Next we will consider the ordering of graphs in $U_n(3)$. Firstly we deal with the trees in $U_n(3)$. With loss of generality we always assume that $a \le b \le c$ for the trees $T(a,b,c)$ in $U_n(3)$.

Theorem 3.2. *For any integer k such that $1 \le k < \lfloor \frac{n-1}{3} \rfloor - 1$, we have that*

$$\rho(T(k, \lfloor \frac{n-k-1}{2} \rfloor, \lceil \frac{n-k-1}{2} \rceil)) < \rho(T(k+1, k+1, n-2k-3)). \quad (4)$$

Proof. To prove the above inequality, we first show the following two equalities.

$$\Phi(T(k+1,k+1,n-2k-3)) = \Phi(P_{k+1})\Phi(\wp_{n-k-1}); \quad (5)$$

$$\Phi(T(k,m,m)) = \Phi(P_m)\Phi(\wp_{k+m+1}). \quad (6)$$

where $\wp_{k+h+1}$ (h is a positive integer) is obtained from a path $P_{k+m+1} = v_1 v_2 \cdots v_k v_{k+1} v_{k+2} \cdots v_{k+h+1}$ by assigning a weight $\sqrt{2}$ to the edge $v_{k+1}v_{k+2}$.

Note that the characteristic polynomial of $T(k+1,k+1,n-2k-3)$ is

$$\begin{vmatrix} xI - A(P_{k+1}) & O & O_1 \\ O & xI - A(P_{k+1}) & O_1 \\ O_1^T & O_1^T & xI - A(P_{n-2k-2}) \end{vmatrix}_{n\times n}$$

where $O_1 = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & \cdots & 0 \end{pmatrix}_{(k+1)\times(n-2k-2)}$

By adding (-1) Row $2(k+1)$ to Row $(k+1)$, then adding Col k and Col $(k+1)$ to Col $(2k+1)$ and Col $2(k+1)$, respectively, we have that $\Phi(T(k+1, k+1, n-2k-3), x)$ equals

$$\begin{vmatrix} xI - A(P_{k+1}) & O_2 & O \\ O & xI - A(P_{k+1}) & O_1 \\ O_1^T & 2O_1^T & xI - A(P_{n-2k-2}) \end{vmatrix}_{n\times n},$$

where $O_2 = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & & \\ 0 & 0 & \cdots & 0 & -1 & 0 \\ 0 & 0 & \cdots & 0 & x & -1 \\ 0 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}_{(k+1)\times(k+1)}.$

After adding (-1) Row $(2k+1)$ and (-1) Row $2k$ to Row k and Row $(k-1)$, respectively, and then adding Col 1 to Col $(k+2)$, the determinant becomes to

$$\begin{vmatrix} xI - A(P_{k+1}) & O & O \\ O & xI - A(P_{k+1}) & O_1 \\ O_1^T & 2O_1^T & xI - A(P_{n-2k-2}) \end{vmatrix}_{n\times n}.$$

By Laplace expansion, it equals to

$$|xI - A(P_{k+1})| \begin{vmatrix} xI - A(P_{k+1}) & O_1 \\ 2O_1^T & xI - A(P_{n-2k-2}) \end{vmatrix}.$$

In the second determinant, first multiplying Col $(k+2)$ by $\sqrt{2}$ and then multiplying Row $(k+2)$ by $\frac{1}{\sqrt{2}}$, we get

$$\begin{vmatrix} xI - A(P_{k+1}) & \sqrt{2}O_1 \\ \sqrt{2}O_1^T & xI - A(P_{n-2k-2}) \end{vmatrix}.$$

So, $\Phi(T(k+1, k+1, n-2k-3)) = \Phi(P_{k+1})\Phi(\wp_{n-k-1})$.

The proof for (6) is similar, and so be omitted.

Now we are ready to prove (4). The proof is divided into two cases depending on the parity of $n-k-1$.

Case 1. $n-k-1$ is even. Then $\lfloor \frac{n-k-1}{2} \rfloor = \lceil \frac{n-k-1}{2} \rceil = \frac{n-k-1}{2}$. According to (6), we have
that $\Phi(T(k, \frac{n-k-1}{2}, \frac{n-k-1}{2})) = \Phi(P_{\frac{n-k-1}{2}})\Phi(\wp_{\frac{n+k+1}{2}})$. Considering the fact

that the largest root of the product of the two polynomials is the larger one between the largest roots of the two polynomials, by Lemma 2.6, it follows that $\rho(T(k, \frac{n-k-1}{2}, \frac{n-k-1}{2})) = \rho(\wp_{\frac{n+k+1}{2}}) < \rho(\wp_{n-k-1}) = \rho(T(k+1, k+1, n-2k-3))$

Case 2. $n-k-1$ is odd. Then $\lfloor\frac{n-k-1}{2}\rfloor = \frac{n-k-2}{2}$, $\lceil\frac{n-k-1}{2}\rceil = \frac{n-k}{2}$. Similar to Case 1, we have that $\Phi(T(k, \frac{n-k}{2}, \frac{n-k}{2})) = \Phi(P_{\frac{n-k}{2}})\Phi(\wp_{\frac{n+k+2}{2}})$. And by Lemma 2.6, $\rho(T(k, \lfloor\frac{n-k-1}{2}\rfloor, \lceil\frac{n-k-1}{2}\rceil)) < \rho(T(k, \frac{n-k}{2}, \frac{n-k}{2})) = \rho(\wp_{\frac{n+k+2}{2}}) < \rho(\wp_{n-k-1}) = \rho(T(k+1, k+1, n-2k-3))$.

This completes the proof of Theorem 3.2. □

The technique used in the proof of Theorem 3.2 is mainly taken from [5]. The following corollary is a stronger result, which gives a complete ordering of all the trees in $U_n(3)$.

Corollary 3.1. $\rho(T(1,1,n-3)) < \rho(T(1,2,n-4)) < \cdots\cdots$
$< \rho(T(1, \lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil)) < \rho(T(2,2,n-5)) < \rho(T(2,3,n-6)) < \cdots\cdots$
$< \rho(T(k, \lfloor\frac{n-k-1}{2}\rfloor, \lceil\frac{n-k-1}{2}\rceil)) < \rho(T(k+1, k+1, n-2k-3))\cdots$
$< \rho(T(\lfloor\frac{n-1}{3}\rfloor - 1, \lfloor\frac{n-\lfloor\frac{n-1}{3}\rfloor}{2}\rfloor, \lceil\frac{n-\lfloor\frac{n-1}{3}\rfloor}{2}\rceil)) < \rho(T(\lfloor\frac{n-1}{3}\rfloor, \lfloor\frac{n-1}{3}\rfloor, m_0))$,

$$\textit{where } m_0 = \begin{cases} \lfloor\frac{n-1}{3}\rfloor & \textit{if } n \equiv 1 \ (mod\ 3); \\ \lceil\frac{n-1}{3}\rceil & \textit{if } n \equiv 2 \ (mod\ 3); \\ \lceil\frac{n-1}{3}\rceil + 1 & \textit{if } n \equiv 0 \ (mod\ 3). \end{cases}$$

Furthermore, if $n \equiv 0$ (mod 3), there is one more inequality to the last one: $\rho(T(\lfloor\frac{n-1}{3}\rfloor, \lfloor\frac{n-1}{3}\rfloor, \lceil\frac{n-1}{3}\rceil + 1)) < \rho(T(\lfloor\frac{n-1}{3}\rfloor, \lceil\frac{n-1}{3}\rceil, \lceil\frac{n-1}{3}\rceil))$.

Proof. Note that $Z_n = T(1,1,n-3)$. From Lemma 2.3, we find that of all the trees in $U_n(3)$, Z_n has the minimal index $\rho(Z_n) = 2cos\frac{\pi}{2(n-1)}$. Other inequalities immediately follows from Lemma 2.1 and Theorem 3.2. □

Now we will present a complete ordering for all the unicyclic graphs in $U_n(3)$.

Theorem 3.3. $\rho(C_{n-1}^{(1)}) < \rho(C_{n-2}^{(2)}) < \cdots < \rho(C_4^{(n-4)}) < \rho(C_3^{(n-3)})$.

Proof. For $k \in \{1, 2, \cdots, n-4\}$, it suffices to show that $\rho(C_{n-k}^{(k)}) < \rho(C_{n-k-1}^{(k+1)})$. Since $C_{n-k}^{(k)}$ can be obtained from $C_{n-k-1}^{(k+1)}$ by subdividing an edge on the cycle C_{n-k-1} and deleting its pendant vertex, by Lemma 2.4 and Lemma 2.6, the above inequality holds. The proof for this theorem is completed. □

How to order all the graphs in $U_n(3)$? Since $T(1, \lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil)$ and $T(\lfloor\frac{n-1}{3}\rfloor, \lfloor\frac{n-1}{3}\rfloor, m_0)$ (where m_0 is as defined in Corollary 3.1) are proper subgraphs of $C_{n-1}^{(1)}$ and $C_{n-\lfloor\frac{n-1}{3}\rfloor}^{(\lfloor\frac{n-1}{3}\rfloor)}$, respectively, we have $\rho(T(1, \lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil))$

$< \rho(C_{n-1}^{(1)})$ and $\rho(T(\lfloor \frac{n-1}{3} \rfloor, \lfloor \frac{n-1}{3} \rfloor, m_0)) < \rho(C_{n-\lfloor \frac{n-1}{3} \rfloor}^{(\lfloor \frac{n-1}{3} \rfloor)})$. Thus the first $\lfloor \frac{n-2}{2} \rfloor$ ones and the last $n-2-\lfloor \frac{n-3}{3} \rfloor$ ones are determined, respectively, in the ordering of $U_n(3)$. But when n is small, $\rho(T(1, \lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil))$ may not be the sharp lower bound for $\rho(C_{n-1}^{(1)})$. By Lemma 2.3, $\rho(T(2,2,2)) = 2$, and $\rho(C_6^{(1)}) > 2$, so it is easy to give a complete ordering of all the graphs in $U_7(3)$. For the other example, by calculation with the software MATLAB, we find that $\rho(T(3,3,3)) = 2.0743 < 2.0785 = \rho(C_9^{(1)})$, and $\rho(T(3,3,4)) = 2.0840 > 2.0743 = \rho(C_{10}^{(1)})$. So, by Theorem 3.2 and 3.3, the complete ordering is determined for all the graphs in $U_{10}(3)$, but the complete ordering is not obtained easily for all the graphs in $U_{11}(3)$. In the general case, not the maximal index of the trees in $U_n(3)$ is always smaller than the minimal one of unicyclic graphs in $U_n(3)$. When $n = 13$, by calculation with MATLAB, we find that $\rho(T(4,4,4)) = 2.1010 > 2.0684 = \rho(C_{12}^{(1)})$, even $\rho(T(2,5,5)) = 2.0840 > \rho(C_{12}^{(1)})$. Generally, by Lemma 2.2 and Remark 2.1, we have the following conclusion.

Corollary 3.2. *When $n > 10$, $\rho(C_{n-1}^{(1)}) > \rho(T(2,2,n-5))$.*

Naturally we will ask : where is the right position for $\rho(C_{n-k}^{(k)})$ in the ordering of all graphs in $U_n(3)$? As a partial result, we give the following conclusion.

Theorem 3.4. *When n is large enough, and k is fixed such that $1 \leq k < \lfloor \frac{n-1}{3} \rfloor - 1$, we have that $\rho(C_{n-k}^{(k)}) < \rho(T(k+1, k+2, n-2k-4))$.*

Proof. By the equation (3) in Section 2, we have $\Phi(T(k+1, k+2, n-2k-4), t^{\frac{1}{2}} + t^{-\frac{1}{2}})t^{n/2}(t-1)^3 = t^{n+3} - 2t^{n+2} + t^{n-k} + t^{n-k-1} + t^{2k+5} - t^{n-2k-2} - t^{k+4} - t^{k+3} + 2t - 1$. Applying Lemma 2.5 to $C_{n-k}^{(k)}$ at that cut edge by which the unique cycle C_{n-k} and the pendant path P_k are linked, we obtain that $\Phi(C_{n-k}^{(k)}) = \Phi(C_{n-k})\Phi(P_k) - \Phi(P_{n-k-1})\Phi(P_{k-1})$. So, by the equations (1) and (2) in Section 2, we get $\Phi(C_{n-k}^{(k)}, t^{\frac{1}{2}} + t^{-\frac{1}{2}})t^{\frac{n}{2}+1}(t-1)^2 = t^{n+3} - 2t^{n+2} + t^{n-k+1} - 2t^{\frac{n+k}{2}+3} + 2t^{\frac{n+k}{2}+2} + 2t^{\frac{n-k}{2}+2} - 2t^{\frac{n-k}{2}+1} + t^{k+3} - 2t^2 + t$. Denote $\Phi(T(k+1, k+2, n-2k-4), t^{\frac{1}{2}} + t^{-\frac{1}{2}})t^{n/2}(t-1)^3$ and $\Phi(C_{n-k}^{(k)}, t^{\frac{1}{2}} + t^{-\frac{1}{2}})t^{\frac{n}{2}+1}(t-1)^2$ by $\Phi_T(t)$ and $\Phi_C(t)$, respectively. Then we have

$$\begin{aligned}\Phi_C(t) - \Phi_T(t) = {} & t^{n-k-1}(t^2 - t - 1) - 2(t-1)(t^{\frac{n+k}{2}+2} - t^{\frac{n-k}{2}+1}) \\ & + t^{k+3}(2 + t - t^{2k+2}) - 2t^2 - t + 1.\end{aligned}$$

Let t_T and t_C be the largest roots of $\Phi_T(t)$ and $\Phi_C(t)$, respectively. Since $C_{n-k}^{(k)}$ contains $C_{n-k}^{(1)}$ as a subgraph, by Lemma 2.6 and Remark 2.1, $t_C > \frac{\sqrt{5}+1}{2}$. Thus $t_C^2 - t_C - 1 > 0$, and $\Phi_C(t_C) - \Phi_T(t_C) > 0$ if n is large enough, and k is fixed such that $1 \leq k < \lfloor \frac{n-1}{3} \rfloor - 1$. Considering

$\Phi_C(t_C) = 0$, we have $\Phi_T(t_C) < 0$, that is, $t_T > t_C$. Note that $\Phi(T(k+1, k+2, n-2k-4), t^{\frac{1}{2}} + t^{-\frac{1}{2}})$ and $\Phi_T(t)$ have the same largest root, so do $\Phi(C_{n-k}^k, t^{\frac{1}{2}} + t^{-\frac{1}{2}})$ and $\Phi_C(t)$. Let $f(t) = t^{\frac{1}{2}} + t^{-\frac{1}{2}}$, then $f'(t) = t^{-\frac{3}{2}}\frac{t-1}{2} \geq 0$ for $t \geq 1$. So $f(t)$ strictly increases in $[1, \infty)$. Therefore, $\rho(C_{n-k}^{(k)}) = t_C^{\frac{1}{2}} + t_C^{-\frac{1}{2}} < t_T^{\frac{1}{2}} + t_T^{-\frac{1}{2}} = \rho(T(k+1, k+2, n-2k-4))$. The proof for Theorem 3.4 is completed. □

By Corollary 3.2 and Theorem 3.4, we can determine the first $n-3(= \lfloor\frac{n-2}{2}\rfloor + \lfloor\frac{n-3}{2}\rfloor)$ ones in the ordering of $U_n(3)$ by their indices: $\rho(T(1,1,n-3)) < \rho(T(1,2,n-4)) < \cdots < \rho(T(1, \lfloor\frac{n-2}{2}\rfloor, \lceil\frac{n-2}{2}\rceil)) < \rho(T(2,2,n-5)) < \rho(C_{n-1}^{(1)}) < \rho(T(2,3,n-6)) < \cdots < \rho(T(2, \lfloor\frac{n-3}{2}\rfloor, \lceil\frac{n-3}{2}\rceil))$. But a large number of computational results suggest that a similar conclusion to corollary 3.2 is also probably true. Therefore we would like to present the following general conjecture.

Conjecture 3.1. *When $n > 10$ is large enough and $k \in \{1, 2, \cdots, \lfloor\frac{n-1}{3}\rfloor - 1\}$ is fixed, we have that $\rho(T(k+1, k+1, n-2k-3)) < \rho(C_{n-k}^{(k)}) < \rho(T(k+1, k+2, n-2k-4))$.*

If the above conjecture is true, the ordering of $U_n(3)$ will be extended to more graphs in this set, and be close to the complete ordering.

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