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On the Skew Spectral Moments of Trees and Unicyclic Graphs

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Abstract Given a simple graph G, the oriented graph G^σ is obtained from G by orienting each edge and G is called the underlying graph of G^σ. The skew-symmetric adjacency matrix $S(G^\sigma)$ of G^σ, where the (u,v)-entry is 1 if there is an arc from u to v, and -1 if there is an arc from v to u (and 0 otherwise), has eigenvalues of 0 or pure imaginary. The k-th-skew spectral moment of G^σ is the sum of power k of all eigenvalues of $S(G^\sigma)$, where k is a non-negative integer. The skew spectral moments can be used to produce graph catalogues. In this paper, we researched the skew spectral moments of some oriented trees and oriented unicyclic graphs and produced their catalogues in lexicographical order. We determined the last $2\lfloor \frac{d}{4}\rfloor$ oriented trees with underlying graph of diameter d and the last $2\lfloor \frac{g}{4}\rfloor+1$ oriented unicyclic graphs with underlying graph of girth g, respectively.

Keywords oriented graph; skew spectral moment; tree; unicyclic graph

MR(2020) Subject Classification 05C50

1. Introduction

Eigenvalues of a graph are found to be widely used in mathematical chemistry, combinatorics, combinatorial optimization and theoretical computer science. Researches about eigenvalues of undirected graphs have a long history [1]. The spectral moments are the sum of power of all eigenvalues. Numerous well-elaborated theories and applications were found in quantum chemistry and solid state physical chemistry. Since the sequence of spectral moments of a graph is an algebraic invariant, the spectral moments can be used to produce graph catalogues. In 1980's, Cvetković et al. studied the mathematical properties of adjacent spectral moments [1–3]. Cvetković and Petrić used spectral moments to produce graph catalogues [4]. In recent years, the adjacent spectral moments are extensively used to produce graph catalogues and more results are obtained [5–12].

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Let G^σ be an oriented graph of G with the orientation σ, which allocates to any edge of G a direction and G is called the underlying graph of G^σ. The skew-adjacency matrix of G^σ is the $n \times n$ matrix $S(G^\sigma) = [s_{ij}]$, where $s_{ij} = 1$ and $s_{ji} = -1$ if v_iv_j is an arc of G^σ, otherwise $s_{ij} = s_{ji} = 0$. Since $S(G^\sigma)$ is skew-symmetric, $iS(G^\sigma)$ is Hermitian and so all of the eigenvalues of $iS(G^\sigma)$ are real. Thus the eigenvalues of $S(G^\sigma)$ are 0 or pure imaginary and since characteristic polynomial of $S(G^\sigma)$ has real coefficients, the eigenvalues occur in complex conjugate pairs.

Recently skew-adjacency matrices of oriented graphs have attracted much attention. Cavers et al. [13] systematically studied skew-adjacency matrices of oriented graphs. Hou and Lei [14] studied the coefficients of the characteristic polynomial of skew-adjacency matrix of an oriented graph. In [15], Shader et al. studied the relationship between the spectra of a graph G and the skew-spectra of an oriented graph G^σ of G. Wong et al. [16] studied relation between the skew-rank of an oriented graph and the rank of its underlying graph. Li et al. [17] studied the skew-rank of an oriented graph and the independence number of its underlying graph. For more results and comprehensive study of the skew-adjacency matrices of oriented graphs, we refer to a survey paper by Cavers et al. [13].

All graphs considered here are finite. Undefined terminology and notation may refer to [18]. Let G^σ be an oriented graph of G with the orientation σ and let $\lambda_1(G^\sigma), \lambda_2(G^\sigma), \ldots, \lambda_n(G^\sigma)$ be the eigenvalues of $S(G^\sigma)$. Note that $\lambda_i(G^\sigma)$ is 0 or pure imaginary, $i = 1, \ldots, n$. The number $\sum_{i=1}^{n} \lambda_i^k(G^\sigma)$ $(k = 0, 1, \ldots, n-1)$, denoted by $T_k(G^\sigma)$, is called the k-th skew spectral moment of G^σ and $T(G^\sigma) = (T_0(G^\sigma), T_1(G^\sigma), \ldots, T_{n-1}(G^\sigma))$ is the sequence of skew spectral moments of G^σ. Suppose $G_1^{\sigma_1}$ and $G_2^{\sigma_2}$ are two digraphs. We shall write $G_1^{\sigma_1} \prec_T G_2^{\sigma_2}$ (G_1 comes before G_2 in a T-order) if for some k $(1 \le k \le n-1)$, $T_i(G_1^{\sigma_1}) = T_i(G_2^{\sigma_2})$ $(i = 0, 1, \ldots, k-1)$ and $T_k(G_1^{\sigma_1}) < T_k(G_2^{\sigma_2})$ holds.

Up to now, few results ordering digraphs by the skew spectral moments are obtained. Taghvaee and Fath-Taber [19] studied the T-order of oriented trees and unicyclic graphs and characterized the first and the last digraphs, in a T-order, of all oriented trees and all oriented unicyclic graphs, respectively. In this paper, we order oriented trees with underlying graph of diameter d and oriented unicyclic graphs with underlying graph of girth g, respectively. By the T-order, we get the last $2\lfloor \frac{d}{4} \rfloor$ oriented trees and the last $2\lfloor \frac{g}{4} \rfloor + 1$ oriented unicyclic graphs, respectively.

2. Preliminaries

In this section, we first give some definitions and lemmas that will be used in the proof of our results.

Let $S(G^\sigma) = [s_{ij}]$ be the skew-adjacency matrix of an oriented graph G^σ and $W = v_1v_2 \cdots v_k$ be a walk from v_1 to v_k. The sign of W is defined as:

$$\mathrm{sgn}(W) = \prod_{i=1}^{k-1} s_{i,i+1}.$$

Let $w_{ij}^+(k)$ and $w_{ij}^-(k)$ denote the number of all positive walks and negative walks starting from v_i and terminating at v_j with length k, respectively, see [20] for more details. Gong and Xu [20] obtained the result about the relationship between the entries of S^k and the number of walks as follows.

Lemma 2.1 ([20]) *Let S be the skew-adjacency matrix of an oriented graph G^σ and v_i and v_j be two arbitrary vertices of G^σ. Then*

$$(S^k)_{ij} = w_{ij}^+(k) - w_{ij}^-(k).$$

Lemma 2.2 ([19]) *The k-th skew spectral moment of G^σ is the number of closed walks with positive sign of length k minus closed walks with negative sign of length k.*

Remark 2.3 Lemma 2.2 is very similar to the following classical result which establishes the relationship between the number of walks and the entries of the power of the adjacency matrix A: the number of walks in G from u to v with length k is equal to $(A^k)_{uv}$.

In an oriented graph G^σ, an even cycle is called evenly oriented if for some choice of direction of traversing around C, the number of edges of C directed in the direction of traversal is even. Otherwise C is called oddly oriented. Throughout this paper, we denote by C_n^+ (or resp., C_n^-) an evenly (or resp., oddly) oriented cycle of order n.

Let $U_{n,g}$ be a graph obtained from C_g by attaching $n-g$ pendant vertices to one vertex of C_g. Denote $U_n = U_{n,n-1}$ and $B_n = K_n - e$. We use U_5^+ (or resp., U_5^-, B_4^+, B_4^-) to denote the oriented graph whose underlying graph is U_5 (or resp., U_5, B_4, B_4) and the longest oriented cycle is C_4^+ (or resp., C_4^-, C_4^+, C_4^-). The graphs U_5^+, U_5^-, B_4^+ and B_4^- are shown in Figure 1.

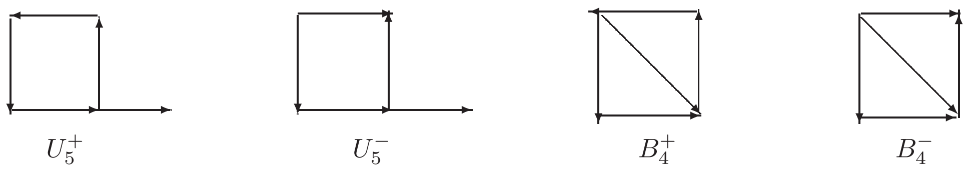

Figure 1 Some oriented graphs U_5^σ and B_4^σ

Let F be a graph. An F-subgraph of G is a subgraph of G which is isomorphic to the graph F. Let $\phi_G(F)$ (or $\phi(F)$) be the number of all F-subgraphs of G.

It is easy to see that $T_0(G^\sigma) = n$, and if k is odd, then $T_k(G^\sigma) = 0$. Taghvaee and Fath-Taber [19] gave the skew spectral moments $T_k(G^\sigma)$ for $k = 2, 4, 6$, respectively.

Lemma 2.4 ([19]) *Let G^σ be an oriented graph. Then we have*

(i) $T_2(G^\sigma) = -2\phi(P_2)$;

(ii) $T_4(G^\sigma) = 2\phi(P_2) + 4\phi(P_3) + 8\phi(C_4^+) - \phi(C_4^-))$;

(iii) $T_6(G^\sigma) = -2\phi(P_2) - 12\phi(P_3) - 6\phi(P_4) - 12\phi(K_{1,3}) + 12(\phi(U_5^-) - \phi(U_5^+)) + 12(\phi(B_4^-) - \phi(B_4^+)) + 24\phi(C_3) + 48(\phi(C_4^-) - \phi(C_4^+)) + 12(\phi(C_6^+) - \phi(C_6^-))$.

Remark 2.5 If G is a graph on n vertices, then we have $\rho(G) \le \rho(K_n) = n-1$ and $\rho_S(G) \le \rho_S(K_n) = \cot\frac{\pi}{2n}$, where $\rho(G)$ and $\rho_S(G)$ are the spectral radius and the skew spectral radius of G, respectively. Since $|E(G)| \leq |E(K_n)| = \binom{n}{2}$, by Lemma 2.4 (i), we have ${K_n}^\sigma \preceq_T G^\sigma$. Fath-Taber [19] proved that ${P_n}^\sigma \preceq_T T^\sigma \preceq_T K_{1,n-1}^\sigma$. So, in a T-order of oriented graphs of order n which the underlying graphs are connected, the first graph is ${K_n}^\sigma$ and the last graph is ${S_n}^\sigma$.

3. Lemmas

Let H_1, H_2 be two connected graphs with $v_i \in V(H_i)$. Let $H_1v_1v_2H_2$ be a graph obtained from H_1, H_2 by identifying v_1 and v_2.

Lemma 3.1 *Let H be a nontrivial connected graph with $w \in V(H)$. Denote $G = HwuK_{1,p+1}$ and $G_1 = HwvK_{1,p+1}$, where u is the pendant vertex of $K_{1,p+1}$ and v is the center of $K_{1,p+1}$, where $p \geq 1$. Then $G^\sigma \prec_T G_1^\sigma$.*

Proof Since $\phi_G(P_2) = \phi_{G_1}(P_2)$, by Lemma 2.4 (i), $T_2(G^\sigma) = T_2(G_1^\sigma)$ holds. Note that $T_i(G^\sigma) = T_i(G_1^\sigma)$ for $i = 0, 1, 2, 3$. Thus we consider the 4-th skew spectral moment of G^σ and G_1^σ, respectively. Note that $\phi_{G^\sigma}(C_4^+) = \phi_{G_1^\sigma}(C_4^+)$, $\phi_{G^\sigma}(C_4^-) = \phi_{G_1^\sigma}(C_4^-)$ and

$$\phi_G(P_3) - \phi_{G_1}(P_3) = \binom{d_H(w)+1}{2} + \binom{p+1}{2} - \binom{d_H(w)+p+1}{2} = -pd_H(w).$$

Then, by Lemma 2.4 (ii), we have

$$T_4(G^\sigma) - T_4(G_1^\sigma) = 2[\phi_G(P_3) - \phi_{G_1}(P_3)] = -2pd_H(w) < 0$$

and $G^\sigma \prec_T G_1^\sigma$. Hence Lemma 3.1 is true. □

Remark 3.2 By Lemma 3.1, for any oriented tree T^σ which is not an oriented star, we can get a tree T'^σ such that $T^\sigma \prec_T T'^\sigma$. So, in T-order, the last graph is the star $K_{1,n-1}^\sigma$ among all oriented trees of order n.

Lemma 3.3 *Let u and v be two vertices of a graph G. The underlying graph $G_{s,t}$ of $G_{s,t}^\sigma$ is obtained by attaching s ($s \geq 1$) pendant vertices $u_1, u_2, \ldots, u_s$ and t ($t \geq 1$) pendant vertices $v_1, v_2, \ldots, v_t$ to u and v, respectively. Then either $G_{s,t}^\sigma \prec_T G_{s+i,t-i}^\sigma$ for $1 \leq i \leq t$ or $G_{s,t}^\sigma \prec_T G_{s-i,t+i}^\sigma$ for $1 \leq i \leq s$ hold.*

Proof Note that $T_i(G_{s,t}^\sigma) = T_i(G_{s+i,t-i}^\sigma) = T_i(G_{s-i,t+i}^\sigma)$ for $i = 0, 1, 2, 3$. Then we will consider the 4-th skew spectral moment of $G_{s,t}^\sigma$, $G_{s+i,t-i}^\sigma$, $G_{s-i,t+i}^\sigma$, respectively. By direct calculation, we have

$$\phi_{G_{s,t}}(P_3) - \phi_{G_{s+i,t-i}}(P_3) = \binom{d_G(u)+s}{2} + \binom{d_G(u)+t}{2} - \binom{d_G(u)+s+i}{2} - \binom{d_G(v)+t-i}{2}$$
$$= (d_G(v) - d_G(u) - s + t - i)i.$$

Since $\phi_{G_{s,t}}(C_4^+) = \phi_{G_{s+i,t-i}}(C_4^+)$ and $\phi_{G_{s,t}}(C_4^-) = \phi_{G_{s+i,t-i}}(C_4^-)$, from Lemma 2.4 (ii), we have

$$T_4(G_{s,t}^\sigma) - T_4(G_{s+i,t-i}^\sigma) = 2[\phi_{G_{s,t}}(P_3) - \phi_{G_{s+i,t-i}}(P_3)] = 2(d_G(v) - d_G(u) - s + t - i)i. \quad (3.1)$$

Similarly,

$$T_4(G_{s,t}^\sigma) - T_4(G_{s-i,t+i}^\sigma) = 2[\phi_{G_{s,t}}(P_3) - \phi_{G_{s-i,t+i}}(P_3)] = 2(d_G(u) - d_G(v) + s - t - i)i. \quad (3.2)$$

If $T_4(G^\sigma_{s,t}) > T_4(G^\sigma_{s+i,t-i})$, by (3.1), then we have $d_G(v) > d_G(u) + s - t + i$. Thus by (3.2), we have $T_4(G^\sigma_{s,t}) - T_4(G^\sigma_{s-i,t+i}) < 2(-2i)i = -4i^2 < 0$. Therefore, $G^\sigma_{s,t} \prec_T G^\sigma_{s-i,t+i}$ holds for $1 \le i \le s$. This completes the proof. □

We give the following notations, which will be used in Lemmas 4.1 and 5.1. A subgraph H of G is called tree-subgraph (or resp., cycle-subgraph) if H is a tree (or resp., contains at least one cycle).

$\mathcal{T}_m(G) = \{T : T$ is a tree-subgraph but not a path of G with $\mathrm{diam}(T) \le \lfloor \frac{m-1}{2} \rfloor + 1\}$;

$\mathcal{P}_m(G) = \{P : P$ is a path-subgraph of G and $|E(P)| \le \lfloor \frac{m}{2} \rfloor + 1\}$;

$\mathcal{C}_m(G) = \{C : C$ is a cycle-subgraph of G and $|E(C)| \le m\}$.

4. T-order of oriented trees

Denote $\mathscr{T}_{n,d} = \{T : T$ is a tree of order n with diameter $d\}$. In the following, we will study the T-order of oriented trees with underlying graph in the set $\mathscr{T}_{n,d}$ for $2 \le d \le n-1$. Cavers et al. [13] found that the skew-adjacency matrices of a graph G are all cospectral if and only if G has no even cycles. Recall that $\mathscr{T}_{n,2} = \{K_{1,n-1}\}$ and $\mathscr{T}_{n,n-1} = \{P_n\}$. Therefore, in the following, we assume that $3 \le d \le n-2$.

In order to formulate our results, we need to define some trees as follows.

Let $T_{n,d}(p_1, \ldots, p_{d-1})$ be a tree of order n created from a path $P_{d+1} = v_1 v_2 \cdots v_d v_{d+1}$ by attaching p_i pendant vertices to v_i, respectively, where $n = d + 1 + \sum_{i=1}^{d-1} p_i$, $p_i \ge 0$, $i = 2, \ldots, d$. Denote $T_{n,d,i} = T_{n,d}(\underbrace{0, \ldots, 0}_{i-1}, n-d-1, 0, \ldots, 0)$. Then $T_{n,d,i} \cong T_{n,d,d-i}$.

Lemma 4.1 *Let $H = v_1 v_2 \cdots v_{n-s}$ be a path of length $n-s-1$. Denote $G = Hv_m uK_{1,s}$, $G_1 = Hv_{m-1}uK_{1,s}$ and $G_2 = Hv_{m+1}uK_{1,s}$, where u is the center of $K_{1,s}$, $3 \le m \le \lfloor \frac{n-s}{2} \rfloor - 1$. Then*

(i) If m is even, then $G_1^\sigma \prec_T G^\sigma$ and $G_1^\sigma \prec_T G_2^\sigma$;

(ii) If m is odd, then $G^\sigma \prec_T G_1^\sigma$ and $G_2^\sigma \prec_T G_1^\sigma$.

Proof Since odd-th skew spectral moments are 0, we only compute $2i$-th skew spectral moments of G^σ and G_l^σ $(l = 1, 2)$, respectively. Note that $\phi_G(P_2) = \phi_{G_l}(P_2)$, by Lemma 2.4 (i), we have $T_2(G^\sigma) = T_2(G_l^\sigma)$ $(l = 1, 2)$. In what follows we compare $T_{2i}(G_l^\sigma)$ and $T_{2i}(G^\sigma)$ $(l = 1, 2)$ for $i \ge 2$. Note that $T_{2i}(G^\sigma)$ $(T_{2i}(G_l^\sigma))$ equals the number of positive closed walks of length $2i$ minus negative closed walks of length $2i$ of $G^\sigma (G_l^\sigma)$. Subgraphs of G (G_l) which can generate closed walks of length $2i$ must be included in $\mathcal{T}_i(G) \bigcup \mathcal{P}_i(G) \bigcup \mathcal{C}_i(G)$ $(\mathcal{T}_i(G_l) \bigcup \mathcal{P}_i(G_l) \bigcup \mathcal{C}_i(G_l)$ $(l = 1, 2)$ for $i \ge 2$.

By the definition of G and G_l $(l = 1, 2)$ for $i \ge 2$, we have

$$\mathcal{C}_i(G_l) = \mathcal{C}_i(G) = \emptyset, \quad \mathcal{P}_i(G_l) = \mathcal{P}_i(G) = \{P_{j+1}, j \le \lfloor \frac{i}{2} \rfloor + 1\},$$

$$\mathcal{T}_i(G_l) = \mathcal{T}_i(G) = \{T_{a,b,t} \text{ for some } a, b, t \text{ such that } a \le \lfloor \frac{i-1}{2} \rfloor + 1, a \le b + 1 + s\}.$$

By direct calculation, we get

$$\phi_G(P_{j+1}) = \phi_{G_l}(P_{j+1}) = \begin{cases} n-1, & \text{if } j=1, \\ \binom{s+2}{2}+n-s-3, & \text{if } j=2, \\ n-j+s, & \text{if } 3\le j\le m-1. \end{cases} \tag{4.1}$$

$$\phi_{G_1}(P_{m+1}) = n-m, \quad \phi_G(P_{m+1}) = \phi_{G_2}(P_{m+1}) = n-m+s \tag{4.2}$$

and for $\forall\, T_{a,b,t} \in \mathcal{T}_i(G)$,

$$\phi_G(T_{a,b,t}) = \phi_{G_l}(T_{a,b,t}) = 2\binom{s}{a-b-1}. \tag{4.3}$$

By (4.1) and (4.3), we have $T_{2i}(G_l^\sigma) = T_{2i}(G^\sigma)$, $i \le m-1$, $l=1,2$.

If m is even, then P_{m+1} generates only positive closed walks of length $2m$ and if m is odd, then P_{m+1} only generates negative closed walks of length $2m$. By Lemma 2.2, (4.1)–(4.3), we get if m is even, then $T_{2m}(G_1^\sigma) < T_{2m}(G^\sigma) = T_{2m}(G_2^\sigma)$, hence $G_1^\sigma \prec_T G^\sigma$ and $G_1^\sigma \prec_T G_2^\sigma$. Thus (i) is true. If m is odd, then $T_{2m}(G_1^\sigma) > T_{2m}(G^\sigma) = T_{2m}(G_2^\sigma)$, hence $G^\sigma \prec_T G_1^\sigma$ and ${G_2}^\sigma \prec_T G_1^\sigma$. Thus (ii) is true. So Lemma 4.1 is true. □

Theorem 4.2 *In a T-order of oriented trees with the underlying graph in the set $\mathscr{T}_{n,d}$, the last $2\lfloor\frac{d}{4}\rfloor$ oriented trees with $3\le d\le n-2$ are as follows:*

$$T^\sigma_{n,d,2}, T^\sigma_{n,d,4}, \ldots, T^\sigma_{n,d,2\lfloor\frac{d}{4}\rfloor}, T^\sigma_{n,d,2\lfloor\frac{d}{4}\rfloor+1}, \ldots, T^\sigma_{n,d,5}, T^\sigma_{n,d,3}.$$

Proof Let T^σ be an oriented tree with underlying graph $T\in\mathscr{T}_{n,d}$. Let $P_{d+1}=v_1v_2\cdots v_dv_{d+1}$ be one of its longest paths of T. By Lemma 3.1, we can get a tree ${T'}^\sigma \cong T^\sigma_{n,d}(a_1,\ldots,a_{d-1})$, where $\sum_{i=1}^{d-1} a_i = n-d-1$ and $T^\sigma \prec_T {T'}^\sigma$. By Lemma 3.3, we can get a tree ${T''}^\sigma \cong T^\sigma_{n,d,i}$ $(2\le i\le d-1)$ and ${T'}^\sigma \prec_T {T''}^\sigma$. Let $H=v_1v_2\cdots v_dv_{d+1}$, star $K_{1,n-d-1}$ with center vertex v, $m=i+1$, then by Lemma 4.1, for $\forall\, i\in[2,\lfloor\frac{d+1}{2}\rfloor-2]$.

(i) If i is even, then $T^\sigma_{n,d,i+1} \prec_T T^\sigma_{n,d,i}$ and $T^\sigma_{n,d,i+2} \prec_T T^\sigma_{n,d,i}$;

(ii) If i is odd, then $T^\sigma_{n,d,i} \prec_T T^\sigma_{n,d,i+1}$ and $T^\sigma_{n,d,i} \prec_T T^\sigma_{n,d,i+2}$.

That is,

$$T^\sigma_{n,d,3} \prec_T T^\sigma_{n,d,5} \prec_T \cdots \prec_T T^\sigma_{n,d,2\lfloor\frac{d}{4}\rfloor+1} \prec_T T^\sigma_{n,d,2\lfloor\frac{d}{4}\rfloor} \prec_T \cdots \prec_T T^\sigma_{n,d,4} \prec_T T^\sigma_{n,d,2}. \quad \square$$

5. T-order of oriented unicyclic graphs

Let $\mathscr{U}_{n,d} = \{G : G \text{ is a unicyclic graph of order } n \text{ with girth } g\}$. In the following, we will study the T-order of oriented unicyclic graphs with underlying graph in the set $\mathscr{U}_{n,g}$ for $3\le g\le n$.

Let $U_{n,g}(p_1,p_2,\ldots,p_{g-1},p_g)$ $(p_i\ge 0)$ be a unicyclic graph of order n created from a cycle $C_g=v_1v_2\cdots v_gv_1$ by attaching p_i leaves to v_i $(i=1,2,\ldots,g)$, respectively, where $n=g+\sum_{i=1}^g p_i$. Denote $U_{n,g}=U_{n,g}(\underbrace{0,\ldots,0}_{g-1},n-g)$ and $U^k_{n,g,i}=U_{n,g}(\underbrace{0,\ldots,0}_{i-1},k,0,\ldots,0,n-g-k)$ for $1\le k\le\lceil\frac{n-g}{2}\rceil$ (see Figure 2). Obviously, $U^k_{n,g,i}\cong U^k_{n,g,g-i}$.

Let $X_{n,g}$ (see Figure 2) be a graph obtained from $U_{n-1,g}$ by attaching a leaf to one leaf of $U_{n-1,g}$.

Let$X_{n,g,k}$ (see Figure 2) be a graph obtained from $U_{n-k-1,g}$ by attaching a leaf of a star $K_{1,k+1}$ ($k \geq 2$) to the maximum vertex of $U_{n-k-1,g}$.

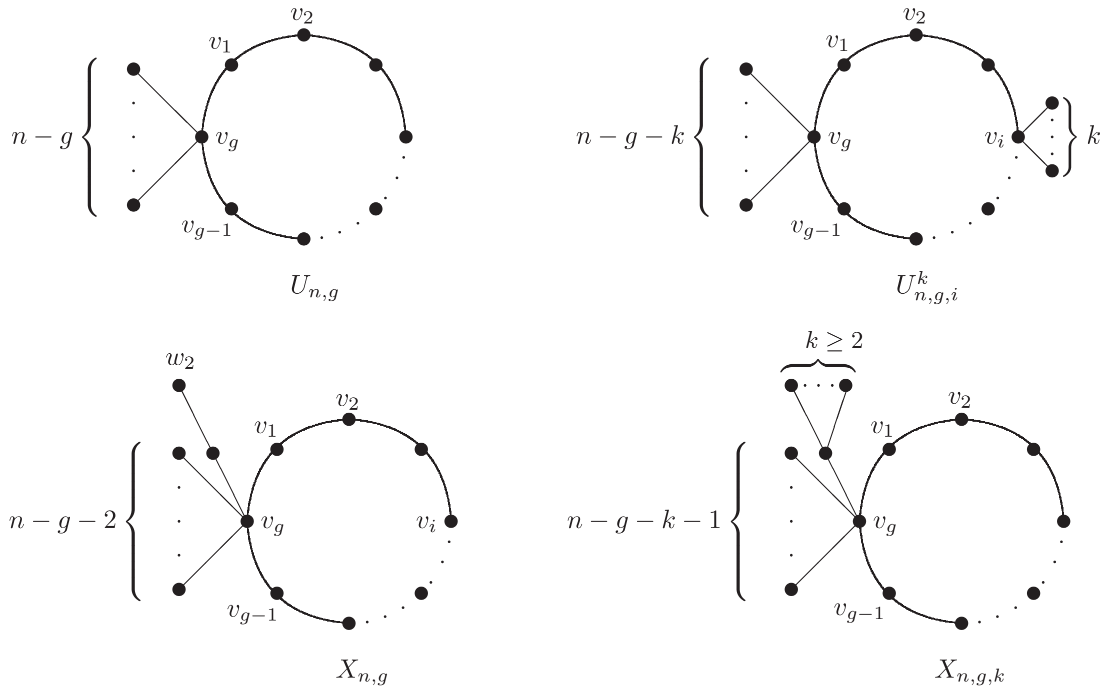

Figure 2 Unicyclic graphs $U_{n,g}$,$U^k_{n,g,i}$,$X_{n,g}$,$X_{n,g,k}$

Remark 5.1 From Lemmas 3.1 and 3.3, in a T-order, the last graph is $U^\sigma_{n,g}$ among all unicyclic graphs of order n with girth g ($g \geq 5$). By Lemma 2.4 (ii), in a T-order, $U^\sigma_{n,4}$ is the last graph of all oriented unicyclic graphs of order n, where the cycle is C_4^+.

Lemma 5.2 *Let $H \cong U_{n-k,g}$ with the unique cycle $C_g = v_1v_2\cdots v_gv_1$. Denote $G = Hv_muK_{1,k}$, $G_1 = Hv_{m-1}uK_{1,k}$ and $G_2 = Hv_{m+1}uK_{1,k}$, where u is the center of $K_{1,k}$, $2 \leq m \leq \lfloor g/2\rfloor - 1$. Then*

(i) If m is even, then $G_1^\sigma \prec_T G^\sigma$ and $G_1^\sigma \prec_T G_2^\sigma$;

(ii) If m is odd, then $G^\sigma \prec_T G_1^\sigma$ and $G_2^\sigma \prec_T G_1^\sigma$.

Proof Note that $T_i(G^\sigma) = T_i(G_l^\sigma) = 0$ when i is odd and $T_j(G^\sigma) = T_j(G_l^\sigma)$ for $j = 0, 2$ and $l = 1, 2$. In what follows, we compare $T_{2i}(G^\sigma)$ and $T_{2i}(G_l^\sigma)$ ($l = 1, 2$) for $i \geq 2$. Similarly, we only need to calculate the numbers of subgraphs included in $\mathcal{T}_i(G)\bigcup\mathcal{P}_i(G)\bigcup\mathcal{C}_i(G)$ ($\mathcal{T}_i(G_l)\bigcup\mathcal{P}_i(G_l)\bigcup\mathcal{C}_i(G_l)$, $l = 1, 2$) for $i \geq 2$.

By the definition of G and G_l ($l = 1, 2$) for $i \geq 2$, we have

$$\mathcal{P}_i(G) = \mathcal{P}_i(G_l) = \{P_{j+1},\ \ j \leq \lfloor\frac{i}{2}\rfloor + 1\},$$

$$\mathcal{C}_i(G)=\mathcal{C}_i(G_l)=\begin{cases}\emptyset, & \text{if } i<g,\\ \{C_g\}, & \text{if } i=g,\\ \{U_{n_1,g},U^{k_1}_{n_2,g,j}\}, & \text{if } i>g.\end{cases}$$

$\mathcal{T}_i(G)=\mathcal{T}_i(G_l)=\{T_{a,b,t}\}\cup\{T'_{a,b,b',t'}$, which is obtained by attaching the center vertex of $K_{1,b'}$ to the t'-th vertex of $T_{a,b,t}, t\neq t', a+b'\le\min\{\lfloor\frac{g}{2}\rfloor,\lfloor\frac{i-1}{2}\rfloor+1\}$, $a-b-1\le n-g-k, b'\le k\}$.

By direct calculation, we get

$$\phi_G(P_{j+1})=\phi_{G_l}(P_{j+1})=\begin{cases}n, & \text{if } j=1,\\ \binom{n-g-k+2}{2}+\binom{k+2}{b}+g-2, & \text{if } j=2,\\ 2n-g, & \text{if } 3\le j\le m,\end{cases}\tag{5.1}$$

$$\phi_{G_1}(P_{m+2})=(n-g-m)(m+2)+2m+g\tag{5.2}$$

and

$$\phi_G(P_{m+2})=\phi_{G_2}(P_{m+2})=2n-g.\tag{5.3}$$

For $\forall\ T_{a,b,t}\in\mathcal{T}_i(G)\ (i\le m+1)$,

$$\phi_G(T_{a,b,t})=\phi_{G_l}(T_{a,b,t})=2\binom{n-g-k}{a-b-1}+2\binom{k}{a-b-1}.\tag{5.4}$$

For $\forall\ T_{a,b,b',t'}\in\mathcal{T}_i(G)\ (i\le m+1)$,

$$\phi_G(T_{a,b,b',t'})=\phi_{G_l}(T_{a,b,b',t'})=\binom{n-g-k}{a-b-1}\binom{k}{b'}.\tag{5.5}$$

By Lemma 2.2, (5.1), (5.4) and (5.5), we have $T_{2i}(G_l^\sigma)=T_{2i}(G^\sigma)$ for $i\le m$ and $l=1,2$. By (5.2) and (5.3), we have $\phi_{G_1}(P_{m+2})>\phi_G(P_{m+2})=\phi_{G_2}(P_{m+2})$. If m is even, since P_{m+2} generates only negative closed walks of length $2(m+1)$, then $T_{2m+2}(G_1^\sigma)<T_{2m+2}(G^\sigma)=T_{2m+2}(G_2^\sigma)$. Hence $G_1^\sigma\prec_T G^\sigma$ and $G_1^\sigma\prec_T G_2^\sigma$. Thus (i) is true. If m is odd, since P_{m+2} generates only positive closed walks of length $2(m+1)$, then $T_{2m+2}(G_2^\sigma)=T_{2m+2}(G^\sigma)<T_{2m+2}(G_1^\sigma)$, hence $G^\sigma\prec_T G_1^\sigma$ and $G_2^\sigma\prec_T G_1^\sigma$. Thus (ii) is true. We have our conclusion. $\square$

For an oriented unicyclic graph, we set $\vec{G}:=G^\sigma$.

Suppose $\vec{G}$ is an oriented unicyclic graph with the underlying graph $G\in\mathscr{U}_{n,g}$. Let $C_g=v_1\cdots v_{g-1}v_g$ be the only cycle of G. Let T_G^i be the component of $G-E(C_g)$ containing v_i $(i=1,2,\ldots,g)$. Obviously, T_G^i is a tree. When $|V(T_G^i)|\ge 2$, we call T_G^i nontrivial.

Theorem 5.3 *In a T-order of oriented unicyclic graphs with the underlying graph in the set $\mathscr{U}_{n,g}$, we have*

(a) If $g\le 5$, then the last $\lfloor\frac{g}{2}\rfloor+1$ oriented unicyclic graphs are as follows:

$$\vec{U}_{n,g},\vec{U}^1_{n,g,2},\vec{U}^1_{n,g,1};$$

(b) If $6\le g\le n-1$ and $g\equiv 3\pmod 4$, then the last $2\lfloor\frac{g}{4}\rfloor+2$ oriented unicyclic graphs are as follows:

$$\vec{U}_{n,g},\vec{U}^1_{n,g,2},\vec{U}^1_{n,g,4},\ldots,\vec{U}^1_{n,g,2\lfloor\frac{g}{4}\rfloor},\vec{U}^1_{n,g,2\lfloor\frac{g}{4}\rfloor+1},\vec{U}^1_{n,g,2\lfloor\frac{g}{4}\rfloor-1},\ldots,\vec{U}^1_{n,g,3},\vec{U}^1_{n,g,1};$$

(c) If $6 \le g \le n-1$ and $g \not\equiv 3 \pmod 4$, then the last $2\lfloor \frac{g}{4} \rfloor + 1$ oriented unicyclic graphs are as follows:

$$\vec{U}_{n,g}, \vec{U}^1_{n,g,2}, \vec{U}^1_{n,g,4}, \ldots, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor}, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor-1}, \ldots, \vec{U}^1_{n,g,3}, \vec{U}^1_{n,g,1}.$$

Proof Suppose $\vec{G}$ is an oriented unicyclic graph with the underlying graph $G \in \mathscr{U}_{n,g}$. First, we suppose only one T^i_G is nontrivial, $i \in \{1, \ldots, g\}$. By Lemma 3.1, we can get an oriented unicyclic graph $\vec{G'} \cong \vec{X}_{n,g,k}$ for some k. By direct calculation, $T_4(\vec{X}_{n,g,k}) < T_4(\vec{X}_{n,g})$ and $T_4(\vec{X}_{n,g}) < T_4(\vec{U}^1_{n,g,i})$. Thus $G \prec_T \vec{X}_{n,g,k} \prec_T \vec{X}_{n,g} \prec_T \vec{U}^1_{n,g,i}$.

Now suppose at least two T^i_G are nontrivial, $i \in \{1, \ldots, g\}$. By Lemma 3.1, we can get an oriented unicyclic graph $\vec{G'} \cong \vec{U}_{n,g}(a_1, \ldots, a_g)$, where $\sum_{i=1}^g a_i = n-g$, and $\vec{G} \prec_T \vec{G'}$. By Lemma 3.3, we can get an oriented unicyclic graph $\vec{G''} \cong \vec{U}^k_{n,g,i}$ $(k \ge 1)$ and then $\vec{G'} \prec_T \vec{G''}$.

Claim 1. $\vec{U}^{k+1}_{n,g,i} \prec_T \vec{U}^k_{n,g,j}$ for $k < \frac{n-g-1}{2}$ and $\forall\, i, j \in \{1, \ldots, g\}$.

Note that $T_l(\vec{U}^{k+1}_{n,g,i}) = T_l(\vec{U}^k_{n,g,j})$ for $l = 0, 1, 2, 3$. By Lemma 2.4 (ii), we have

$$T_4(\vec{U}^{k+1}_{n,g,j}) - T_4(\vec{U}^k_{n,g,i}) = 4(n-g-2k-1) > 0.$$

Hence Claim 1 is true.

(a) Since $3 \le g \le 5$, by Lemmas 2.4 (i) and (ii), $T_l(\vec{U}^k_{n,g,1}) = T_l(\vec{U}^k_{n,g,2})$ for $l = 0, 1, \ldots, 5$. By Lemma 2.4 (iii), we have

$$T_6(\vec{U}^k_{n,g,1}) - T_6(\vec{U}^k_{n,g,2}) = -6k(n-g-k) < 0.$$

Hence if $g \le 5$, then $\vec{U}^k_{n,g,1} \prec_T \vec{U}^k_{n,g,2}$. By Lemma 3.3, $\vec{U}^k_{n,g,2} \prec_T \vec{U}_{n,g}$. By Claim 1, when $g \le 5$, the last $\lfloor \frac{g}{2} \rfloor + 1$ oriented unicyclic graphs are as follows:

$$\vec{U}_{n,g}, \vec{U}^1_{n,g,2}, \vec{U}^1_{n,g,1}.$$

Let $H = U_{n-k,g}$, $K_{1,k}$ be a star with center vertex v. By Lemma 5.2, we have the following claim.

Claim 2. For $k \le \frac{n-g}{2}$, $g \ge 6$ and $2 \le i \le \lfloor \frac{g}{2} \rfloor$, we have

(i) If i is odd, then $\vec{U}^k_{n,g,i} \prec_T \vec{U}^k_{n,g,i-1}$ and $\vec{U}^k_{n,g,i+1} \prec_T \vec{U}^k_{n,g,i-1}$;

(ii) If i is even, then $\vec{U}^k_{n,g,i-1} \prec_T \vec{U}^k_{n,g,i}$ and $\vec{U}^k_{n,g,i-1} \prec_T \vec{U}^k_{n,g,i+1}$.

(b) By Claim 2 (i), we have

$$\vec{U}^k_{n,g,2} \succ_T \vec{U}^k_{n,g,4} \succ_T \cdots \succ_T \vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor}.$$

By Claim 2 (ii), we have

$$\vec{U}^k_{n,g,1} \prec_T \vec{U}^k_{n,g,3} \prec_T \cdots \prec_T \vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor-1}.$$

By Claim 2 (ii), we have $\vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor-1} \prec_T \vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor}$. By simple caculation, we have

$$\begin{cases} U^k_{n,g,2\lfloor \frac{g}{4} \rfloor+1} \cong U^k_{n,g,2\lfloor \frac{g}{4} \rfloor-1}, & \text{if } g \equiv 0 \pmod 4, \\ U^k_{n,g,2\lfloor \frac{g}{4} \rfloor+1} \cong U^k_{n,g,2\lfloor \frac{g}{4} \rfloor-1}, & \text{if } g \equiv 1 \pmod 4, \\ U^k_{n,g,2\lfloor \frac{g}{4} \rfloor+1} \cong U^k_{n,g,2\lfloor \frac{g}{4} \rfloor}, & \text{if } g \equiv 2 \pmod 4, \\ U^k_{n,g,2\lfloor \frac{g}{4} \rfloor+1} \ncong U^k_{n,g,i}, & \text{if } g \equiv 3 \pmod 4. \end{cases} \qquad (*)$$

By Claim 1, when $k \geq 2$, we have $\vec{U}^k_{n,g,i} \prec_T \vec{U}^1_{n,g,2}$ ($2 \leq i < \lfloor \frac{g}{2} \rfloor$). By Lemma 3.3, $\vec{U}^1_{n,g,1} \prec_T \vec{U}_{n,g}$ holds. If $6 \leq g \leq n-1$ and $g \equiv 3 \pmod 4$, by (∗), then $U^k_{n,g,2\lfloor \frac{g}{4} \rfloor+1} \ncong U^k_{n,g,i}$, where $i \neq 2\lfloor \frac{g}{4} \rfloor + 1$. By (i) and (ii), we have $\vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor-1} \prec_T \vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor+1} \prec_T \vec{U}^k_{n,g,2\lfloor \frac{g}{4} \rfloor}$. Hence the last $2\lfloor \frac{g}{4} \rfloor + 2$ oriented unicyclic graphs are as follows:

$$\vec{U}_{n,g}, \vec{U}^1_{n,g,2}, \vec{U}^1_{n,g,4}, \ldots, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor}, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor+1}, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor-1}, \ldots, \vec{U}^1_{n,g,3}, \vec{U}^1_{n,g,1}.$$

(c) If $6 \leq g \leq n-1$ and $g \not\equiv 3 \pmod 4$, by (∗), then the last $2\lfloor \frac{g}{4} \rfloor + 1$ oriented unicyclic graphs are as follows:

$$\vec{U}_{n,g}, \vec{U}^1_{n,g,2}, \vec{U}^1_{n,g,4}, \ldots, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor}, \vec{U}^1_{n,g,2\lfloor \frac{g}{4} \rfloor-1}, \ldots, \vec{U}^1_{n,g,3}, \vec{U}^1_{n,g,1}.$$

This completes the proof. □

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References

[1] D. CVETKOVIĆ, M. DOOB, H. SACHS. *Spectra of Graphs Theory and Applications*. Academic Press, New York, 1980.

[2] D. CVETKOVIĆ, M. DOOB, H. SACHS, et al. *Recent Results in the Theory of Graph Spectra*. North-Holland Publishing Co., Amsterdam, 1988.

[3] D. CVETKOVIĆ, P. ROWLINSON. *Spectra of unicyclic graphs*. Graphs Combin., 1987, **3**(1): 7–23.

[4] D. CVETKOVIĆ, M. PETRIC. *A table of connected graphs on six vertices*. Discrete Math., 1984, **50**(1): 37–49.

[5] Yaping WU, Huiqing LIU. *Lexicographical ordering by spectral moments of trees with a prescribed diameter*. Linear Algebra Appl., 2010, **433**(11-12): 1707–1713.

[6] Xiangfeng PAN, Xiaolan HU, Xiuguo LIU, et al. *The spectral moments of trees with given maximum degree*. Appl. Math. Lett., 2011, **24**(7): 1265–1268.

[7] Xiangfeng PAN, Xiuguo LIU, Huiqing LIU. *On the spectral moment of quasi-trees*. Linear Algebra Appl., 2012, **436**(5): 927–934.

[8] Bo CHENG, Bolian LIU. *Lexicographical ordering by spectral moments of trees with k pendant vertices and integer partitions*. Appl. Math. Lett., 2012, **25**(5): 858–861.

[9] Bo CHENG, Bolian LIU, Jianxi LIU. *On the spectral moments of unicyclic graphs with fixed diameter*. Linear Algebra Appl., 2012, **437**(4): 1123–1131.

[10] E. ANDRIANTIANA, S. WAGNER. *Spectral moments of trees with given degree sequence*. Linear Algebra Appl., 2013, **439**(12): 3980–4002.

[11] Shuchao LI, Huihui ZHANG, Mingjie ZHANG. *On the spectral moment of graphs with K cut edges*. Electron. J. Linear Algebra, 2013, **26**: 718–731.

[12] Shuchao LI, Jiajia ZHANG. *Lexicographical ordering by spectral moments of trees with a given bipartition*. Bull. Iranian Math. Soc., 2014, **40**(4): 1027–1045.

[13] M. CAVERS, S. M. CIOABA, S. FALLAT, et al. *Skew adjacency matrices of graphs*. Linear Algebra Appl., 2012, **436**(12): 5412–5429.

[14] Yaoping HOU, Tiangang LEI. *Charteristic polynominal of skew-adjacency matrices of orinted graphs*. Elec. J. Combin., 2011, **18**: 156–167.

[15] B. SHADER, W. SO. *Skew spectra of oriented graphs*. Elec. J. Combin., 2009 **16**: 1–6.

[16] Dein WONG, Xiaobin MA, Fenglei TIAN. *Relation between the skew-rank of an oriented graph and the rank of its underlying graph*. European J. Combin., 2016, **54**: 76–86.

[17] Xueliang LI, Wen XIA. *Skew rank of an oriented graph and independence number of its underlying graph*. J. Comb. Optim., 2019, **38**(1): 268–277.

[18] J. A. BONDY, U. S. R. MURTY. *Graph Theory with Applications*. Macmillan, London, 1976.

[19] F. TAGHVAEE, G. H. FATH-TABAR. *On the skew spectral moments of graphs*. Trans. Comb., 2017, **6**(1): 47–54.

[20] Shicai GONG, Guanghui XU. *3-Regular digraphs with optimum skew energy*. Linear. Algebra. Appl., 2012, **436**(3): 465–471.