

On k -trees with Extremal Signless Laplacian Estrada Index and Estrada Index

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Abstract The signless Laplacian Estrada index $SLEE(G)$ (resp. Estrada index $EE(G)$) of a graph G is defined as $SLEE(G) = \sum_{i=1}^n e^{q_i}$ (resp. $EE(G) = \sum_{i=1}^n e^{\lambda_i}$). Let T_n^k be the set of the k -trees of order n . In this paper , by the methods on power series in mathematical analysis and spectral moment in algebra graph theory , the pseudo-order on the two indices was obtained. Further by contradiction , the extremal graphs among T_n^k having the first , the second largest signless Laplacian Estrada index (resp. Estrada index) were characterized.

Keywords k -tree; signless Laplacian Estrada index; Estrada index

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k -树的极值无符号的拉普拉斯 Estrada 指标和 Estrada 指标

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摘要 图 G 的无符号的拉普拉斯 Estrada 指标 $SLEE(G)$ (Estrada 指标 $EE(G)$) 定义为 $SLEE(G) = \sum_{i=1}^n e^{q_i}$ ($EE(G) = \sum_{i=1}^n e^{\lambda_i}$)。设 T_n^k 为 n 阶 k -树的集合。利用数学分析中幂级数和代数图论中谱距的方法, 建立了这两类指标的伪序。结合反证法, 刻画了 T_n^k 中具有第一、第二最大的无符号的拉普拉斯 Estrada 指标 (Estrada 指标) 的极值图。

关键词 k -树; 无符号拉普拉斯 Estrada 指标; Estrada 指标

All graphs considered in this paper are finite , undirected and simple. Let $G=(V, E)$ be a connected graph , let $N_G(v) = \{u | uv \in E\}$, $N_G[v] = N_G(v) \cup \{v\}$. Denote $d_G(v) = |N_G(v)|$ by the degree of the vertex v of G . If $W \subset V$, let $N_G(W) = \cup_{v \in W} N_G(v) \setminus W$, $N_G[W]$ be the set of vertices within distance at most 1 from W , $G-W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. If $E_0 \subset E(G)$, we denote by $G-E_0$ the subgraph of G obtained by deleting the edges in E_0 . If E_1 is the subset of the edge set of the complement of G , $G+E$ denotes the graph obtained from G by adding the edges in E_1 : If E

$= \{xy\}$ and $W = \{v\}$, we write $G-xy$ and $G-v$ instead of $G-\{xy\}$ and $G-\{v\}$, respectively. The join $G_1 \vee G_2$ of two edge-disjoint graphs G_1 and G_2 is obtained by adding an edge from each vertex in G_1 to each vertex in G_2 . For other undefined notations we refer to Bollobás^[1].

The adjacency matrix $A=A(G)$ of G is a matrix whose (i, j) -th entry is equal to 1 if vertices v_i and v_j are adjacent , and 0 otherwise. Since A is a real symmetric matrix , its eigenvalues are real numbers. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be the eigenvalues of adjacency matrix A . Let $M_k(G)$ be the k th spectral moment of the

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graph G , i. e., $M_k(G) = \sum_{i=1}^n \lambda_i^k$. The Estrada index, put forward by Estrada^[2], is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i} = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}$.

Let $D = D(G) = \text{diag}(d(v_1), \dots, d(v_n))$ be a diagonal matrix with degrees of the corresponding vertices of G on the main diagonal and zero elsewhere, where $d(v_i)$ is the degree of v_i . The matrix $Q = D(G) + A(G)$ is called the signless Laplacian of G . Since Q is real symmetric and positive semi-definite matrix, its eigenvalues are real numbers. Let $q_1 \geq q_2 \geq \dots \geq q_n \geq 0$ are the signless Laplacian eigenvalues of G . The multiplicity of 0 as an eigenvalue of Q is equal to the number of bipartite connected components of G . The set of all eigenvalues of Q is the signless Laplacian spectrum of G .

A semi-edge walk (of length k) in a graph G is an alternating sequence $v_1, e_1, v_2, e_2, \dots, v_k, e_k, v_{k+1}$ of vertices v_1, v_2, \dots, v_{k+1} and edges e_1, e_2, \dots, e_k such that for any $i = 1, 2, \dots, k$ the vertices v_i and v_{i+1} are end-vertices (not necessarily distinct) of the edge e_i . From Ref [3], we know that the (i, j) -entry of the matrix Q^k is equal to the number of semi-edge walks of length k starting at vertex v_i and terminating at vertex v_j . Let

$T_k = \sum_{i=1}^n q_i^k = \text{Tr}(Q^k)$ be the k -th spectral moment for Q , that is, T_k is equal to the number of closed semi-edge walks of length k . Then the signless Laplacian Estrada index $SLEE(G)$, which is introduced by Ayyaswamy S K, et al in Ref [4], of a graph G can be

$$SLEE(G) = \sum_{i=1}^n e^{q_i} = \sum_{k=0}^{\infty} \frac{T_k}{k!}.$$

As an extension of trees, the k -tree is defined as either a complete graph on k vertices or a graph obtained from a smaller k -tree by adjoining a new vertex together with k edges connecting it to a $k+1$ -clique. Let T_n^k be the set of all n -vertex k -trees.

Since Harary and Palmer^[5] first introduced 2-trees in 1968, Beineke and Pippert^[6] gave the definition of a k -tree in 1969, the study of properties on k -trees arouse many researchers interest. For examples, Estes J and Wei B^[7] obtained the sharp bounds of the Zagreb indices of k -trees. In Ref [8],

Wang S and Wei B characterized the extremal graphs and determined the exact bounds of multiplicative Zagreb indices of k -trees, which attain the lower and upper bounds. In Ref [9], Wang X X, et al attained the upper bounds on the spectral radius of k -trees. Huang F and Wang S^[10] characterized the graphs among T_n^k having the first (resp. the second) largest Estrada index, and so on. In this note, we will give a unified approach, which is simpler than the one used in Ref [10], to characterize the graphs among T_n^k having the first, the second largest signless Laplacian Estrada index (resp. Estrada index).

1 Preliminaries

In this section, we give some definitions and structure properties of k -trees which will be used in the proof of our main results.

Let T_n^k be a k -tree. If v is a vertex of T_n^k with degree k whose neighbours form a k -clique, then v is called a k -simplicial vertex. We use $S_1(T_n^k)$ for the set of all simplicial vertices of T_n^k , when $n \geq k + 2$. Set $S_1(K_k) = \emptyset$ and $S_1(K_{k+1}) = \{v\}$, where v is any vertex of K_{k+1} .

Lemma 1^[11]

- (i) $S_1(T_n^k) \neq \emptyset$ for $n \geq k + 1$.
- (ii) $S_1(T_n^k)$ is an independent set when $n \geq k + 1$.
- (iii) $T_n^k - S_1(T_n^k)$ is a k -tree and every k -simplicial vertex (if any) of $T_n^k - S_1(T_n^k)$ is adjacent in T_n^k to at least one vertex of $S_1(T_n^k)$.

Let K_k be a k -clique and S be an independent set of $n - k$ vertices. $A(k; n)$ -star, denoted by $S_{k, n-k}$, is defined as $S_{k, n-k} = K_k \vee S$ (as shown in Fig. 1). Let $S'_{k, n-k} = S_{k, n-k} - u_1 v_1 + u_1 u_2$.

Lemma 2^[10] Let T_n^k be a k -tree of order n . If $|S_1(T_n^k)| = n - k$, then it is a $(k; n)$ -star.

Let G and H be two graphs with $u_1, v_1 \in V(G)$ and $u_2, v_2 \in V(H)$. If $M_k(G; u_1, v_1) \leq M_k(H; u_2, v_2)$ for all positive integers k , then we write $(G; u_1, v_1) \leq M(H; u_2, v_2)$. If $(G; u_1, v_1) \leq M(H; u_2, v_2)$ and there is at least one positive integer k_0 such that $M_{k_0}(G; u_1, v_1) < M_{k_0}(H; u_2, v_2)$; then we write $(G; u_1, v_1) < M(H; u_2, v_2)$. Similarly, if $T_k(G; u_1, v_1) \leq T_k(H; u_2, v_2)$,

v_2) for all positive integers k , then we write $(G; u_1, v_1) \leq T(H; u_2, v_2)$. If $(G; u_1, v_1) \leq T(H; u_2, v_2)$ and there is at least one positive integer k_0 such that $T_{k_0}(G;$

$u_1, v_1) < T_{k_0}(H; u_2, v_2)$; then we write $(G; u_1, v_1) < T(H; u_2, v_2)$. If $u_i = v_i$, we write $(G; u_i, v_i)$ as $(G; u_i)$ for $i = 1, 2, \dots$.

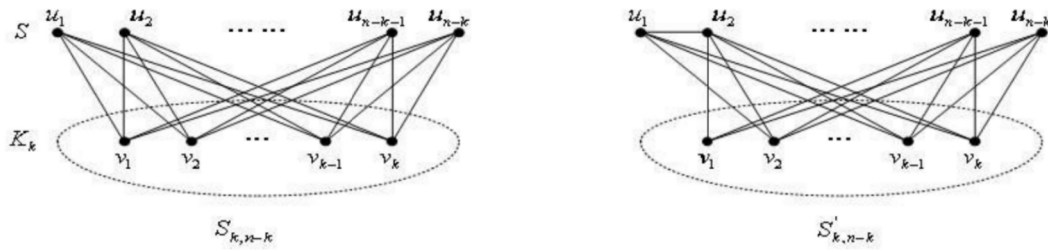


Fig.1 The k -trees $S_{k, n-k}$ and $S'_{k, n-k}$

图 1 k -树 $S_{k, n-k}$ 和 $S'_{k, n-k}$

Lemma 3 Let $u, v \in V(G)$ and $N_G(v) \subseteq N_G[u]$. Then

(i) $(G; v) \leq M(G; u)$ and $(G; w, v) \leq M(G; w, u)$ for each $w \in V(G)$. Moreover, if $d_G(v) < d_G(u)$ then $(G; v) < M(G; u)$.

(ii) $(G; v) \leq T(G; u)$, and $(G; w, v) \leq T(G; w, u)$ for each $w \in V(G)$ ^[12]. Moreover, if $d_G(v) < d_G(u)$ then $(G; v) < T(G; u)$.

Proof We only need to prove (i).

Firstly, we prove $(G; v) \leq M(G; u)$.

Let W be a walk in $W_k(G; v)$. If u is not in W , note that $N_G(v) \subseteq N_G[u]$, let $f(W) = W'$, where W' is the walk that is obtained by replacing the vertex v by u , obviously, $W' \in W_k(G; u)$. If u is in W , we can also look W as a walk which is starting and ending at vertex u , let $f(W) = W$.

Obviously, f is an injection from $W_k(G; v)$ to $W_k(G; u)$. Hence $(G; v) \leq M(G; u)$. If $d_G(v) < d_G(u)$, f is not a surjection, then $(G; v) < T(G; u)$.

Secondly, we prove $(G; w, v) \leq M(G; w, u)$ for each $w \in V(G)$. If \tilde{W} be a walk in $W_k(G; w, v)$, let $\tilde{f}(\tilde{W}) = \tilde{W}'$, where \tilde{W}' is the walk which is obtained by replacing the vertex v by u . \tilde{f} is also an injection $W_k(G; w, v)$ to $W_k(G; w, u)$, we have $(G; w, v) \leq M(G; w, u)$ for each $w \in V(G)$.

Lemma 4 Let G be a graph and $v, u, w_1, w_2, \dots, w_r \in V(G)$. Suppose that $E_v = \{e_1 = vw_1, \dots, e_r = vw_r\}$ and $E_u = \{e'_1 = uw_1, \dots, e'_r = uw_r\}$, where $e_i, e'_i \notin E(G)$, for $i = 1, 2, \dots, r$. Let $G_u = G + E_u$ and $G_v = G + E_v$.

(i) If $(G; v) < T(G; u)$, and $(G; w_i, v) \leq M(G; w_i, u)$ for each $i = 1, 2, \dots, r$ then $EE(G_v) < EE(G_u)$ ^[13].

(ii) If $(G; v) < T(G; u)$, and $(G; w_i, v) \leq T(G; w_i,$

$u)$ for each $i = 1, 2, \dots, r$, then $SLEE(G_v) < SLEE(G_u)$ ^[14].

Lemma 4 is an excellent tool to deal with the extremal problems on Estrada index and signless Laplacian Estrada index, but it has many conditions which have to be provided when we want to use it. The lemma 3 enables us to discover a special case that provides such conditions.

2 Main results

In this section, we will give a unified method to characterize the k -trees with the largest and second largest Estrada index and signless Laplacian Estrada index, respectively, which is simpler than the method provided in Ref [10].

Lemma 5 Let G be a graph with $vu, uv \in E(G)$ and $vw \notin E(G)$. Let $G' = G - vu + vw$. If $N_G(v) \subseteq N_G[u]$, then $EE(G) < EE(G')$ and $SLEE(G) < SLEE(G')$.

Proof Let $H = G - vu$. Then $G = H + vu$; $G' = H + vw$ and $N_H(v) \subseteq N_H[u]$. Note that $w \notin N_G[v]$, we have $d_H(v) < d_H(u)$. By Lemma 3, we have $(H; w, v) \leq B(H; w, u)$ for each $w \in V(H)$ and $(H; v) < B(H; u)$, where $B \in \{M, T\}$. Further by Lemma 4, we have $EE(G) < EE(G')$ and $SLEE(G) < SLEE(G')$.

Repeated by Lemma 5, we can obtain the following result.

Lemma 6 Let G be a graph and $X = \{x_1, x_2, \dots, x_t\}$ be an independent set of equivalent vertices such that $x_i u, uv \in E(G)$ and $x_i w \notin E(G)$ for $1 \leq i \leq t$. Let $G' = G - \{x_i u, 1 \leq i \leq t\} + \{x_i w, 1 \leq i \leq t\}$. If $N_G(v) \subseteq N_G[u]$, then $EE(G) < EE(G')$ and $SLEE(G) < SLEE(G')$.

Lemma 7 For a graph $G \in T_n^k$, if there exists a

vertex $v \in S_1(G - S_1(G))$, then there is a graph $G' \in T_n^k$ such that $|S_1(G')| = |S_1(G)| + 1$, $EE(G) < EE(G')$ and $SLEE(G) < SLEE(G')$.

Proof Since there exists a vertex $v \in S_1(G - S_1(G))$, let $N_{G-S_1(G)}(v) = \{v_1, v_2, \dots, v_k\}$, $U_C(v) = N_G(v) - N_{G-S_1(G)}(v)$. Then the vertices in $N_{G-S_1(G)}(v)$ induce a complete graph K_k ; and the vertices in $U_C(v)$ which are all simplicial vertices, induce an empty graph.

For a vertex $x \in U_C(v)$, it is adjacent to all but one vertex in $N_{G-S_1(G)}(v)$. Let U_i be the set of vertices in $U_C(v)$ whose neighbour set is $P_C(v) = |\{1 \leq i \leq k, U_i \neq \emptyset\}|$, where $1 \leq i \leq k$. For a vertex $v \in S_1(G - S_1(G))$, let $v \in S_1(G - S_1(G))$ and $p(G) = \min\{|P_C(v) \cap S_1(G - S_1(G))|\}$. Without loss of generality, let $p_C(u) = p(G)$, $N_{G-S_1(G)}(v) = \{v_1, v_2, \dots, v_k\}$ and $U_C(u) = U_1 \cup \dots \cup U_{p(G)}$ (as shown in Fig. 2). Obviously, we have $N_G[U_i] \subseteq N_G[u]$ for $1 \leq i \leq k$. Let $G' = G - \{ux : x \in U_1\} + \{v_1x : x \in U_1\}$.

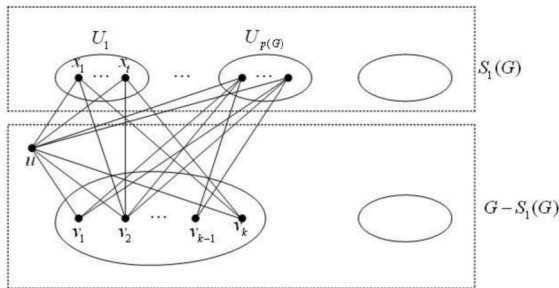


Fig.2 The structure of $N_{G-S_1(G)}(v)$ and $U_C(u)$

图 2 $N_{G-S_1(G)}(v)$ 和 $U_C(u)$ 的结构

Note that $v_1x \notin E(G)$. By Lemma 6, we have $EE(G) < EE(G')$ and $SLEE(G) < SLEE(G')$. Obviously $S_1(G') = S_1(G) \cup \{u\}$, and $|S_1(G')| = |S_1(G)| + 1$. This completes the proof.

Repeatedly by Lemma 7, we can see that the k -tree T_n^k which has the largest Estrada index and signless Laplacian Estrada index satisfies $S_1(T_n^k - S_1(T_n^k)) = \emptyset$. Further by lemmas 1 and 2, we have $T_n^k \cong S_{k, n-k}$. Then we have the following theorem.

Theorem 1 For any $T_n^k \in T_n^k$, $EE(T_n^k) < EE(S_{k, n-k})$ and $SLEE(T_n^k) < SLEE(S_{k, n-k})$. The equality holds if and only if $T_n^k \cong S_{k, n-k}$.

In the following, we consider the graphs with the second largest Estrada index and signless Laplacian

Estrada index in T_n^k .

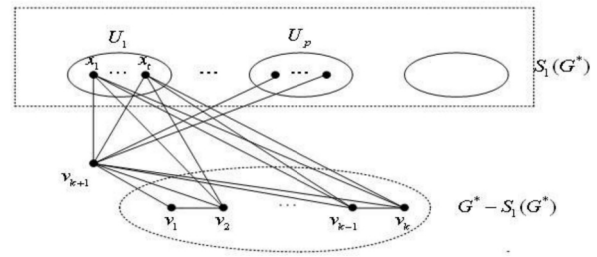


Fig.3 The structure of the graph G^* in the proof in Theorem 9

图 3 定理 9 证明中图 G^* 的结构

Theorem 2 For any $T_n^k \in T_n^k \setminus S_{k, n-k}$, $EE(T_n^k) \leq EE(S'_{k, n-k})$ and $SLEE(T_n^k) \leq SLEE(S'_{k, n-k})$. The equality holds if and only if $T_n^k \cong S'_{k, n-k}$.

Proof Let G^* be the graph in $T_n^k \setminus S_{k, n-k}$ whose Estrada index and signless Laplacian Estrada index is as larger as possible. By Lemma 7, we have $|S_1(G^* - S_1(G^*))| = 1$, that is $G^* - S_1(G^*) \cong K_{k+1}$.

Let $V(G^*) \setminus S_1(G^*) = \{v_1, v_2, \dots, v_{k+1}\}$ and $|S_1(G^* - S_1(G^*))| = \{v_{k+1}\}$. Further, let $U_C(v_{k+1}) = N_G(v_{k+1}) - \{v_1, v_2, \dots, v_k\}$; U_i be the set of vertices in $U_C(v_{k+1})$ whose neighbour set is $\{v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_k, v_{k+1}\}$ for $1 \leq i \leq k$, and $p = |\{1 \leq i \leq k, U_i \neq \emptyset\}|$ (as shown in Fig.3).

Case 1 $p \geq 2$, let $G_1 = G^* - \{v_{k+1}x : x \in U_1\} + \{v_1x : x \in U_1\}$. Obviously $G_1 \in T_n^k \setminus S_{k, n-k}$. By Lemma 6, we have $EE(G_1) > EE(G^*)$ and $SLEE(G_1) > SLEE(G^*)$, a contradiction.

Case 2 $p = 1$ and $S_1(G^*) - U_C(v_{k+1}) = \emptyset$, then $G^* \cong S_{k, n-k}$ it is contradict to $G^* \in T_n^k \setminus S_{k, n-k}$.

Case 3 $p = 1$ and $S_1(G^*) - U_C(v_{k+1}) = \emptyset$.

If $|U_1| \geq 2$, let $U_1 = \{x_1, \dots, x_i\}$ and $G_2 = G^* - v_{k+1}x_1 + v_1x_1$. Obviously, $G_2 \in T_n^k \setminus S_{k, n-k}$. By Lemma 5, we have $EE(G_2) > EE(G^*)$ and $SLEE(G_2) > SLEE(G^*)$, a contradiction.

If $|U_1| = 1$, we have $G^* \cong S'_{k, n-k}$.

Case 4 $p = 0$, then $G^* \cong S_{k, n-k}$, it is contradict to $G^* \in T_n^k \setminus S_{k, n-k}$.

This completes the proof.

For any $T_n^k \in T_n^k$, if $k = 1$, then T_n^k is the ordinary tree. Let T_n^k be the class of trees of order n . Let S_n and S'_n be the graphs as shown in Fig.4. Then by theorems 1 and 2, we have the following results.

Corollary Let $T \in T_n \setminus \{S_n, S'_n\}$. Then

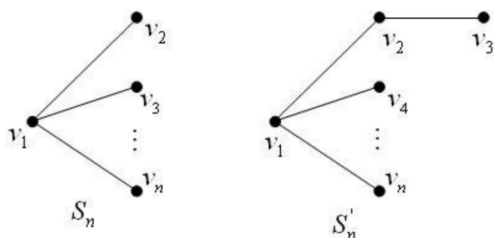


Fig.4 The graphs S_n and S'_n

图 4 图 S_n 和 S'_n

- (i) $EE(T) < EE(S'_n) < EE(S_n)$ [5].
- (ii) $SLEE(T) < SLEE(S'_n) < SLEE(S_n)$.

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