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A Note on the Maximal Estrada Index of Trees with a Given Bipartition

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Abstract

Let G be a simple graph with n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix. The Estrada index EE of G is the sum of the terms e^{λ_i}. Let $\mathcal{T}(p,q)$ denote the set of all trees with a given (p,q)-bipartition, where $q \geq p \geq 2$. And $D(p,q)$ denotes the double star which is obtained by joining the centers of two stars S_p and S_q by an edge. In this note, we will show that $D(p,q)$ has the maximal Estrada index in $\mathcal{T}(p,q)$.

1 Introduction

Let G be a simple graph with n vertices, the spectrum of G is the spectrum of its adjacency matrix [1], and consists of the (real) numbers $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The Estrada index is defined as

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

In our proof, we will use a relation between EE and the spectral moments of a graph. For $k \geq 0$, we denote by M_k the k-th spectral moment of G, $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$. We know from [1] that M_k is equal to the number of closed walks of length k in the graph G.

By the Taylor expansion of e^x, we have the following important relation between the Estrada index and the spectral moments of G:

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k}{k!}.$$

Thus, if for two graphs G and H we have $M_k(G) \geq M_k(H)$ for all $k \geq 0$, then $EE(G) \geq EE(H)$. Moreover, if the strict inequality $M_k(G) > M_k(H)$ holds for at least one value of k, then $EE(G) > EE(H)$.

Recently, Deng in [2] showed that the path P_n and the star S_n have the minimal and the maximal Estrada indices among n-vertex trees. In 2010, J. Li et al. [3] obtained the trees with minimal Estrada index among trees of order n with exactly two vertices of maximum degree. Let $\mathcal{T}(p,q)$ denote the set of all trees with a given (p,q)-bipartition, where $q \geq p \geq 2$. And $D(p,q)$ denotes the double star which is obtained by joining the centers of two stars S_p and S_q by an edge. In this note, we will show that $D(p,q)$ has the maximal Estrada index in $\mathcal{T}(p,q)$.

2 The maximal Estrada index of trees with a given bipartition

The coalescence $G(u) \cdot H(v)$ of rooted graphs G and H is the graph obtained from G and H by identifying the root u of G with the root v of H. Let $W_k(G)$ be the set of closed walks of length k in G, $W_k(G,u)$ denote the set of closed walks of length k starting at u in G, and $M_k(G) = |W_k(G)|$, $M_k(G,u) = |W_k(G,u)|$.

Lemma 2.1 *[4] If G_1 and G_2 are the bipartite graphs satisfying $M_{2k}(G_1) \geq M_{2k}(G_2)$ and $M_{2k}(G_1,w) \geq M_{2k}(G_2,u)$ for any positive integer k, then $M_{2k}(G) \geq M_{2k}(G')$ for any positive integer k, where $G \cong G_1(w) \cdot G_3(a)$ and $G' \cong G_2(u) \cdot G_3(a)$ (see Fig. 1). Furthermore, if $M_{2k}(G_1,w) > M_{2k}(G_2,u)$ for some positive integer k, then there must exist a positive integer l such that $M_{2l}(G) > M_{2l}(G')$.*

Figure 1. The graphs considered in Lemma 2.1..

Now we are ready to prove our main result:

Theorem 2.2 *If* $T \in \mathcal{T}(p,q)$, $q \geq p \geq 2$, *and* $T \ncong D(p,q)$, *then* $EE(T) < EE(D(p,q))$.

Proof. Let s denote the number of pendent vertices of T, we prove the theorem by induction on s.

Let $p+q=n$. If $s=n-1$, then the tree must be the star S_n, a contradiction.

If $s=n-2$, then the longest path in T must be P_4, and other edges are pendent edges on the second or the third vertices of the path. Since it has a given (p,q)-bipartition, the tree can only be $D(p,q)$.

Let $2 \leq l \leq n-3$, and suppose that the result holds for $s > l$. Now we consider $s = l$. Letting $P = v_1v_2\cdots v_t$ be an arbitrary path in T, then T can be repainted as T' in Fig.2, where T_i is the tree planting at v_i, $1 \leq i \leq t$, and $T_1 \neq K_1$. T'' is the tree from T' by exchanging the position of T_1 from v_1 to v_3, so the pendent edges of T'' is $l+1$. Now we prove that $EE(T') < EE(T'')$. By Lemma 2.1, we only need to prove that $M_{2k}(T', v_1) \leq M_{2k}(T'', v_3)$.

For any closed walk $w' \in W_{2k}(T', v_1)$, it contains the first segments w'_1 which is the edge v_1v_2, the second segment w'_2 from the first v_2 to the last v_2, and the third segment w'_3 which is the last edge v_2v_1. Then, define another walk w'' in $W_{2k}(T'', v_3)$, where the first segments w''_1 is the edge v_3v_2, the second segment w''_2 is exactly w'_2, and the third segment w''_3 is the last edge v_2v_3.

Now, for any closed walk $w' \in W_{2k}(T', v_1)$, there is a unique walk $w'' \in W_{2k}(T'', v_3)$ corresponding to it. Clearly the correspondence is injective, but not surjective. Thus we have $M_{2k}(T', v_1) \leq M_{2k}(T'', v_3)$.

Let V_1, V_2 be the bipartition of vertex set of T', with $|V_1| = p$ and $|V_2| = q$. We can see that the bipartition is all the same in T'' as in T'.

By the induction hypothesis $EE(T'') < EE(D(p,q))$, therefore we have $EE(T) < EE(D(p,q))$. ∎

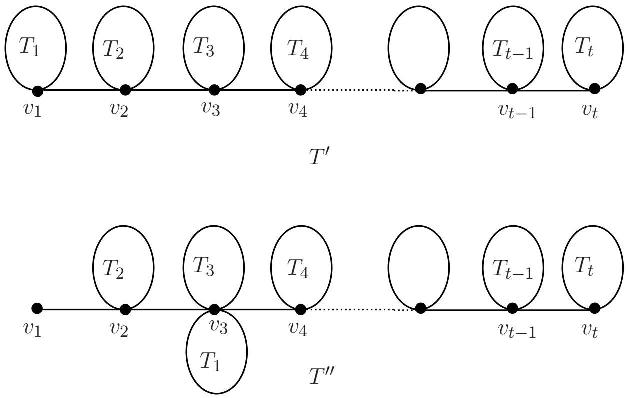

Figure 2. The trees in the proof of Theorem 2.2.

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