The Estrada index of trees
Zhibin Du\textsuperscript{a}, Bo Zhou\textsuperscript{b,*}

\textsuperscript{a} Department of Mathematics, Tongji University, Shanghai 200092, China
\textsuperscript{b} Department of Mathematics, South China Normal University, Guangzhou 510631, China

A B S T R A C T

The Estrada index of a graph $G$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of its adjacency matrix. We determine the unique tree with maximum Estrada index among the set of trees with given number of pendant vertices. As applications, we determine trees with maximum Estrada index among the set of trees with given matching number, independence number, and domination number, respectively. Finally, we give a proof of a conjecture in [J. Li, X. Li, L. Wang, The minimal Estrada index of trees with two maximum degree vertices, MATCH Commun. Math. Comput. Chem. 64 (2010) 799–810] on trees with minimum Estrada index among the set of trees with two adjacent vertices of maximum degree.

© 2011 Elsevier Inc. All rights reserved.

1. Introduction

Let $G$ be a simple graph with vertex set $V(G)$. The eigenvalues of $G$ are the eigenvalues of its adjacency matrix $A(G)$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, where $n = |V(G)|$, see [2]. The Estrada index of a graph $G$ is defined as [5]

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$
The Estrada index has been successfully employed to quantify the degree of folding of long-chain molecules, especially proteins [5–7], and to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks [8,9]. There is also a connection between the Estrada index and the extended atomic branching of molecules [10]. Until now lots of properties of the Estrada index have been established. Various bounds for the Estrada index can be found in [3,11,12,15,17–19]. See [4,13,14,16] for more results. We know that the star $S_n$ is the unique $n$-vertex tree with maximum Estrada index [4,11,19], and the path $P_n$ is the unique $n$-vertex tree with minimum Estrada index [4]. Ilič and Stevanović [15] determined the unique tree with minimum Estrada index among the set of trees with given maximum degree. Zhang et al. [17] determined the unique tree with maximum Estrada indices among the set of trees with given matching number. Li et al. [16] determined the unique tree with minimum Estrada index among the set of trees with exactly two vertices of maximum degree, and they also proposed the following conjecture.

**Conjecture 1.1** [16]. Among the set of $n$-vertex trees with two adjacent vertices of maximum degree $\Delta$, where $n \geq 2\Delta + 1 \geq 7$, the tree obtained by adding an edge between the centers of two stars $S_\Delta$, and attaching a path on $n - 2\Delta$ vertices (at an end vertex) to a pendant vertex is the unique tree with minimum Estrada index.

In this paper, we determine the unique tree with maximum Estrada index among the set of trees with given number of pendant vertices (vertices of degree one). As applications, we determine trees with maximum Estrada index among the set of trees with given matching number, independence number, and domination number, respectively. Finally, we give a proof of Conjecture 1.1.

**2. Preliminaries**

Denote by $M_k(G)$ the $k$th spectral moment of the graph $G$, i.e., $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$. It is well-known that $M_k(G)$ is equal to the number of closed walks of length $k$ in $G$ [2]. Then

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

In particular, if $G$ is a bipartite graph, then $M_{2k+1}(G) = 0$ for $k \geq 0$, and thus

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_{2k}(G)}{(2k)!}.$$ 

Let $M_k(G; u)$ be the number of (closed) $(u, u)$-walks of length $k$ in the graph $G$.

Let $G_1$ and $G_2$ be bipartite graphs. If $M_{2k}(G_1) \geq M_{2k}(G_2)$ for all positive integers $k$, then we write $G_1 \succeq G_2$. If $G_1 \succeq G_2$ and there is at least one positive integer $k_0$ such that $M_{2k_0}(G_1) > M_{2k_0}(G_2)$, then we write $G_1 \succ G_2$. By above expression for the Estrada index, $G_1 \succeq G_2$ implies that $EE(G_1) \geq EE(G_2)$, and $G_1 \succ G_2$ implies that $EE(G_1) > EE(G_2)$. Let $u \in V(G_1)$ and $v \in V(G_2)$. If $M_{2k}(G_1; u) \geq M_{2k}(G_2; v)$ for all positive integers $k$, then we write $(G_1; u) \succeq (G_2; v)$. If $(G_1; u) \succ (G_2; v)$ and there is at least one positive integer $k_0$ such that $M_{2k_0}(G_1; u) > M_{2k_0}(G_2; v)$, then we write $(G_1; u) > (G_2; v)$.

We give some lemmas that will be used later.

**Lemma 2.1** [17]. Let $G$ and $H$ be two vertex-disjoint bipartite graphs with $u, v \in V(G)$ and $w \in V(H)$, where $|V(H)| \geq 2$. Let $GuH$ be the graph obtained from $G$ and $H$ by identifying $u$ with $w$, and $GvH$ the graph obtained from $G$ and $H$ by identifying $v$ with $w$. If $(G; u) > (G; v)$, then $GuH > GvH$.

**Lemma 2.2** [15]. Let $w$ be a vertex of the nontrivial connected graph $G$. For non-negative integers $p$ and $q$, let $G_{p,q}$ be the graph obtained from $G$ by attaching two paths, respectively, on $p$ vertices and $q$ vertices to $w$. If $p \geq q \geq 1$, then $EE(G_{p,q}) > EE(G_{p+1,q-1})$. 

For two vertices \( u, v \) of a graph \( G \), let \( \mathcal{W}_k(G; u, [v]) \) be the set of \((u, u)\)-walks of length \( k \) containing \( v \) in \( G \). Let \( M_k(G; u, [v]) = |\mathcal{W}_k(G; u, [v])| \).

### 3. Estrada index of trees with given parameters

A pendant path at a vertex \( v \) of a graph \( G \) is a path in \( G \) connecting vertex \( v \) and a pendant vertex such that all internal vertices (if exist) in this path have degree two and the degree of \( v \) is at least three.

Let \( d_G(u, v) \) be the distance between vertices \( u \) and \( v \) in the connected graph \( G \).

For an edge \( uv \) of the edge set of the graph \( G \), \( G - uv \) denotes the graph obtained from \( G \) by deleting the edge \( uv \), and for an edge \( uv \) of the edge set of the complement of \( G \), \( G + uv \) denotes the graph obtained from \( G \) by adding the edge \( uv \).

**Lemma 3.1.** Let \( G \) and \( G_1 \) be connected bipartite graphs in Fig. 1, where the path from \( v \) to \( w \) in \( G \) is a pendant path at \( v \), and all neighbors of \( v \) in \( Q \) of \( G \) are switched to be neighbors of \( u \) in \( Q \) of \( G_1 \). If \( d_G(v, w) \leq \max \{d_G(u, x) : x \in V(S)\} \) and \( S \) is not a path with an end vertex \( u \), then \( EE(G) < EE(G_1) \).

**Proof.** Let \( H \) be the graph obtained from \( G \) by deleting the vertices of \( Q \). Let \( P \) be the path from \( v \) to \( w \) in \( G \). Let \( k \) be any positive integer.

Since \( d_G(v, w) \leq \max \{d_G(u, x) : x \in V(S)\} \), there is a vertex \( z \in V(S) \) such that \( d_G(v, w) \leq d_G(u, z) \), i.e., \( d_P(v, w) \leq d_S(u, z) \). Since \( S \) is not a path with an end vertex \( u \), \( P \) is a proper subgraph of \( S \), and then \( (S; u) \succ (P; v) \).

For \( W \in \mathcal{W}_{2k}(H; u, [v]) \), we may decompose \( W \) into \( W = W_1W_2 \), where \( W_1 \) is the shortest \((u, v)\)-section (consisting of a \((u, u)\)-walk in \( S \) whose length may be zero and a single edge \( uv \)) of \( W \), and \( W_2 \) is the remaining \((v, u)\)-section of \( W \). For \( x, y \in V(H) \), let \( r_s(H; x, y) \) be the number of \((x, y)\)-walks of length \( s \) in \( H \). Thus

\[
M_{2k}(H; u, [v]) = \sum_{\substack{k_1 + k_2 = 2k \\ k_1, k_2 \geq 1 \\ k_1, k_2 \text{ are odd}}} M_{k_1-1}(S; u) r_{k_2}(H; v, u).
\]

Similarly,

\[
M_{2k}(H; v, [u]) = \sum_{\substack{k_1 + k_2 = 2k \\ k_1, k_2 \geq 1 \\ k_1, k_2 \text{ are odd}}} M_{k_1-1}(P; v) r_{k_2}(H; u, v).
\]

Obviously, \( r_s(H; v, u) = r_s(H; u, v) \) for any positive integer \( s \), see [2]. Thus \( M_{2k}(H; u, [v]) \geq M_{2k}(H; v, [u]) \).

Note that

\[
M_{2k}(H; u) = M_{2k}(H; u, [v]) + M_{2k}(S; u)
\]

and

\[
M_{2k}(H; v) = M_{2k}(H; v, [u]) + M_{2k}(P; v).
\]

Then \((H; u) \succ (H; v)\). Now the result follows from Lemma 2.1. □

![Fig. 1. The graphs \( G \) and \( G_1 \) in Lemma 3.1.](image-url)
Let $T(n, p)$ be the set of trees with $n$ vertices and $p$ pendant vertices, where $2 \leq p \leq n - 1$.

Let $n$, $p$ be positive integers. Let $s = \lceil \frac{n-1}{p} \rceil$, $r = n - 1 - ps$. Let $T_{n,p}$ be the tree obtained by attaching $p - r$ paths on $s$ vertices and $r$ paths on $s + 1$ vertices to a single vertex, where $2 \leq p \leq n - 1$.

**Theorem 3.1.** Let $G \in T(n, p)$, where $2 \leq p \leq n - 1$. Then $EE(G) \leq EE(T_{n,p})$ with equality if and only if $G \cong T_{n,p}$.

**Proof.** The cases $p = 2$, $n - 1$ are trivial. Suppose that $3 \leq p \leq n - 2$.

Let $G$ be a tree in $T(n, p)$ with maximum Estrada index. Let $V_1(G)$ be the set of vertices of $G$ with degree at least three. Let $P$ be a pendant path with minimum length in $G$ at a vertex $v$ in $V_1(G)$, and $w$ be the pendant vertex of $G$ in $P$.

Suppose that $|V_1(G)| \geq 2$. Choose a vertex $y$ in $V_1(G)$ such that $d_G(v, y)$ is as small as possible. Then the internal vertices (if exist) of the unique path connecting $v$ and $y$ in $G$ are of degree two. Denote by $u$ the neighbor of $v$ in $G$ lying on the path connecting $v$ and $y$ $(u = y$ if $v$ and $y$ are adjacent in $G$). Let $S$ be the component of $G - v$ containing $y$. Obviously, $S$ is not a path with an end vertex $u$. By the choice of $P$, we have $d_G(u, w) \leq \max\{d_G(u, x) : x \in V(S)\}$. Applying Lemma 3.1 to $G$, we may get a tree $G_1 \in T(n, p)$ such that $EE(G) < EE(G_1)$, a contradiction. Thus $|V_1(G)| = 1$, i.e., $v$ is the unique vertex in $G$ with degree at least three. If $G \not\cong T_{n,p}$, then by Lemma 2.2, we have $EE(G) < EE(T_{n,p})$, a contradiction. It follows that $G \cong T_{n,p}$. □

**Lemma 3.2.** For $2 \leq p \leq n - 2$, $EE(T_{n,p}) < EE(T_{n,p+1})$.

**Proof.** Let $u$ be the pendant vertex of a longest pendant path in $T_{n,p}$. Let $v$ be the neighbor of $u$ and $w$ the neighbor of $v$ different from $u$ in $T_{n,p}$. By Lemma 2.2, $EE(T_{n,p}) < EE(T_{n,p} - uv + uw)$. Note that there are $p + 1$ pendant vertices in $T_{n,p} - uv + uw$. By Theorem 3.1, $EE(T_{n,p} - uv + uw) \leq EE(T_{n,p+1})$.

The result follows easily. □

A matching $M$ of the graph $G$ is an edge subset of $G$ such that no two edges in $M$ share a common vertex. The matching number of $G$ is the maximum cardinality of a matching of $G$.

For $2 \leq r \leq \lfloor n/2 \rfloor$, let $T^{n,r}$ be the tree obtained by attaching $r - 1$ paths on two vertices to the center of the star $S_{n-2r+2}$.

The following result has been given in [17]. Now we give a different proof.

**Corollary 3.1** [17]. Let $G$ be a tree with $n$ vertices and matching number $m$, where $2 \leq m \leq \lfloor n/2 \rfloor$. Then $EE(G) \leq EE(T^{n,m})$ with equality if and only if $G \cong T^{n,m}$.

**Proof.** Let $M$ be a matching in $G$ with $|M| = m$. Let $p$ be the number of pendant vertices in $G$. Obviously, there is at most one pendant end vertex for an edge of $M$. Then $p \leq m + (n - 2m) = n - m$.

If $p = n - m$, then by Theorem 3.1 (with $s = 1$ and $r = m - 1$), we have $T^{n,m} \cong T_{n,n-m}$ is the unique tree with maximum Estrada index. If $p < n - m$, then by Theorem 3.1 and Lemma 3.2, $EE(G) \leq EE(T_{n,p}) < \cdots < EE(T_{n,n-m}) = EE(T^{n,m})$. The result follows. □

An independent set is a vertex subset in which no pair is adjacent. The independence number of a graph $G$, denoted by $\alpha(G)$, is the maximum cardinality of an independent set of $G$. It is well-known that in any bipartite graph $G$, the sum of the independence number of $G$ and the matching number of $G$ is equal to the number of vertices of $G$, see [1]. From Corollary 3.1, we have

**Corollary 3.2.** Let $G$ be a tree with $n$ vertices and independence number $\alpha = \alpha(G)$, where $\lfloor n/2 \rfloor \leq \alpha \leq n - 2$. Then $EE(G) \leq EE(T^{n,n-\alpha})$ with equality if and only if $G \cong T^{n,n-\alpha}$.

A dominating set of a graph is a subset of vertices whose closed neighborhood includes all vertices of the graph. The domination number of a graph $G$, denoted by $\gamma(G)$, is the minimum cardinality of a dominating set.
Lemma 3.3 (König’s theorem [1]). Let \( G \) be a bipartite graph. Then the matching number of \( G \) is equal to the minimum cardinality of a covering of \( G \).

Corollary 3.3. Let \( G \) be a tree with \( n \) vertices and domination number \( \gamma = \gamma(G) \), where \( 2 \leq \gamma \leq \lfloor n/2 \rfloor \). Then \( EE(G) \leq EE(T(n, \gamma)) \) with equality if and only if \( G \cong T(n, \gamma) \).

Proof. Let \( m \) be the matching number of \( G \). It is easily seen that a covering of \( G \) is also a dominating set of \( G \). By Lemma 3.3, \( m \geq \gamma \). If \( m = \gamma \), then by Corollary 3.1, \( EE(G) \leq EE(T(n, \gamma)) \) with equality if and only if \( G \cong T(n, \gamma) \). If \( m > \gamma \), then by Corollary 3.1 and Lemma 2.2, \( EE(G) \leq EE(T(n, m)) < EE(T(n, m-1)) < \cdots < EE(T(n, \gamma)) \). The result follows. \( \square \)

4. Estrada index of trees with two adjacent vertices of maximum degree

For integer \( r \geq 1 \), let \( H_{r:p,q} \) be the tree obtained by attaching paths \( P : u_1u_2 \ldots u_p \) and \( Q : v_1v_2 \ldots v_q \) at end vertices \( u_1 \) and \( v_1 \) to the center \( w \) of a star on \( r + 1 \) vertices, where \( p \geq q \geq 1 \).

Lemma 4.1. If \( p > q \geq 1 \), then \( (H_{r:p,q}; u_1) > (H_{r:p,q}; v_1) \).

Proof. Let \( H_{p,q} = H_{r:p,q} \). Let \( k \) be a positive integer. Note that
\[
M_{2k}(H_{p,q}; u_1) = M_{2k}(P; u_1) + M_{2k}(H_{p,q}; u_1, [w])
\]
and
\[
M_{2k}(H_{p,q}; v_1) = M_{2k}(Q; v_1) + M_{2k}(H_{p,q}; v_1, [w])
\]
Since \( p > q \geq 1 \), \( Q \) is a proper subgraph of \( P \), and then \( (P; u_1) > (Q; v_1) \). Thus we need only to show that
\[
M_{2k}(H_{p,q}; u_1, [w]) \geq M_{2k}(H_{p,q}; v_1, [w])
\]
We construct a mapping \( f \) from \( \mathcal{W}_{2k}(H_{p,q}; u_1, [w]) \) to \( \mathcal{W}_{2k}(H_{p,q}; v_1, [w]) \). For \( W \in \mathcal{W}_{2k}(H_{p,q}; v_1, [w]) \), we may decompose \( W \) into \( W = W_1W_2W_3 \), where \( W_1 \) is the shortest \((v_1, w)\)-section in \( W \) (for which the internal vertices, if exist, are only possible to be \( v_1, v_2, \ldots, v_q \), \( W_2 \) is the longest \((w, w)\)-section in \( W \) whose length may be zero, and \( W_3 \) is the remaining \((w, v_1)\)-section of \( W \) (for which the internal vertices, if exist, are only possible to be \( v_1, v_2, \ldots, v_q \)). Let \( f(W) = f(W_1)f(W_2)f(W_3) \), where \( f(W_1) \) is a \((u_1, w)\)-walk obtained from \( W_1 \) by replacing \( v_1 \) by \( u_i \) for \( i = 1, 2, \ldots, q \), \( f(W_2) = W_2 \) and \( f(W_3) \) is a \((w, u_1)\)-walk obtained from \( W_3 \) by replacing \( v_1 \) by \( u_i \) for \( i = 1, 2, \ldots, q \). Obviously, \( f(W) \in \mathcal{W}_{2k}(H_{p,q}; u_1, [w]) \) and \( f \) is an injection. Thus \( M_{2k}(H_{p,q}; v_1, [w]) \leq M_{2k}(H_{p,q}; u_1, [w]) \). \( \square \)

For integer \( r \geq 1 \), let \( G_{r:p,q} \) be the tree obtained from a path \( P = uv \) by attaching \( r \) pendant vertices and a path on \( p \) vertices to \( u \), and attaching \( r \) pendant vertices and a path on \( q \) vertices to \( v \), where \( p \geq q \geq 1 \).

Lemma 4.2. For positive integers \( p, q \) with \( p \geq q \geq 2 \), we have \( EE(G_{r:p,q}) > EE(G_{r:p+1,q-1}) \).

Proof. It is easily seen that \( G_{r:p,q} (G_{r:p+1,q-1}, \text{respectively}) \) can be obtained from \( H_{r:p+1,q} \) and \( S_{r+1} \) with center \( w \) by identifying \( u_1 \in V(H_{r:p+1,q}) \) (\( v_1 \in V(H_{r:p+1,q}), \text{respectively} \)) with \( w \in V(S_{r+1}) \). Note that \( p + 1 > q \). By Lemma 4.1, \( (H_{r:p+1,q}; u_1) > (H_{r:p+1,q}; v_1) \). Now by Lemma 2.1, we have \( G_{r:p,q} > G_{r:p+1,q-1} \). The result follows. \( \square \)

Let \( D_{n, \Delta} \) be the tree obtained by adding an edge between the centers of two vertex-disjoint stars \( S_{\Delta} \), and attaching a path on \( n - 2\Delta \) vertices to a pendant vertex, where \( n \geq 2\Delta + 1 \geq 7 \).
Theorem 4.1. Let \( G \) be an \( n \)-vertex tree with two adjacent vertices of maximum degree \( \Delta \), where \( n \geq 2\Delta + 1 \geq 7 \). Then \( EE(G) \geq EE(D_{n,\Delta}) \) with equality if and only if \( G \cong D_{n,\Delta} \).

Proof. Let \( G \) be a tree with minimum Estrada index among \( n \)-vertex trees with two adjacent vertices, say \( u \) and \( v \) of maximum degree \( \Delta \). By Lemma 2.2, we have \( G \cong G_{r;p,q} \), where \( r = \Delta - 2, p \geq q \geq 1 \), and \( p + q = n - 2\Delta + 2 \). If \( q \geq 2 \), then by Lemma 4.2, \( EE(G) = EE(G_{r;p,q}) > EE(G_{r;p+1,q-1}) \), a contradiction. Thus \( q = 1 \) and \( p = n - 2\Delta + 1 \), i.e., \( G \cong D_{n,\Delta} \). □

This proves Conjecture 1.1.

5. Concluding remark

It remains an open problem to determine the tree(s) with minimum Estrada index among the set of trees with given parameters such as number of pendant vertices or matching number.

Acknowledgement

This work was supported by the National Natural Science Foundation of China (Grant No. 11071089).

References