Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

ON THE ESTRADA INDEX OF GRAPHS WITH GIVEN NUMBER OF CUT EDGES*

ZHIBIN DU† AND BO ZHOU‡

Abstract. Let G be a simple graph with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. The Estrada index of G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. In this paper, the unique graph with maximum Estrada index is determined among connected graphs with given numbers of vertices and cut edges.

Key words. Estrada index, Cut edge, Spectral moments, Pendant vertex.

AMS subject classifications. 05C50, 05C35, 05C90, 15A18.

1. Introduction. Let G be a simple graph with n vertices. The eigenvalues of the adjacency matrix $\mathbf{A}(G)$ of G are called the eigenvalues of G, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$. The Estrada index of a graph G is defined as

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

This concept was proposed in [4], and it found successful applications in biochemistry and in complex networks, see [4–9]. Besides these applications, the Estrada index has also been extensively studied in mathematics, see [2, 3, 10, 11, 13–15]. Among these, Ilić and Stevanović [11] determined the unique tree with minimum Estrada index among the set of trees with given maximum degree. Zhang et al. [13] determined the unique tree with maximum Estrada index among the set of trees with given matching number.

A cut edge of a connected graph is an edge whose removal disconnects the graph. For $0 \le r \le n-3$, let $\mathbb{G}(n,r)$ be the set of connected graphs with n vertices and r cut edges, and $G_{n,r}$ the graph obtained by attaching r pendant vertices (vertices of degree one) to a vertex of K_{n-r}, where K_n is the complete graph on n vertices. Liu et al. [12] characterized the unique graph in $\mathbb{G}(n,r)$ with maximum spectral radius,

*Received by the editors on December 14, 2010. Accepted for publication on May 20, 2011. Handling Editor: Bryan Shader. This work was supported by National Natural Science Foundation of China (Grant No. 11071089).

†Department of Mathematics, Tongji University, Shanghai 200092, P.R. China (zhibindu@126.com).

‡Department of Mathematics, South China Normal University, Guangzhou 510631, P.R. China (zhoubo@scnu.edu.cn).

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

which is $G_{n,r}$. In this paper, we determine the unique graph in $\mathbb{G}(n,r)$ with maximum Estrada index, which is also $G_{n,r}$.

2. Preliminaries. Denote by $M_k(G)$ the kth spectral moment of 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, see [1]. Then

$$EE(G) = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!} = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \tag{2.1}$$

Let $V(G)$ be the vertex set of G. Let $M_k(G; u)$ be the number of closed walks of length k starting at u in G.

Let G_1 and G_2 be two graphs. If $M_k(G_1) \leq M_k(G_2)$ for all positive integers k, then by (2.1), we have $EE(G_1) \leq EE(G_2)$ with equality if and only if $M_k(G_1) = M_k(G_2)$ for all positive integers k. Let $u \in V(G_1)$ and $v \in V(G_2)$. If $M_k(G_1; u) \leq M_k(G_2; v)$ for all positive integers k, then we write $(G_1; u) \preceq (G_2; v)$. If $(G_1; u) \preceq (G_2; v)$ and there is at least one positive integer k_0 such that $M_{k_0}(G_1; u) < M_{k_0}(G_2; v)$, then we write $(G_1; u) \prec (G_2; v)$.

Let $d_G(v)$ be the degree of vertex v in the graph G.

For a vertex u of a graph G, $G - u$ denotes the graph obtained from G by deleting u and its incident edges. For subset S of the edge set of a graph G, $G - S$ denotes the graph obtained from G by deleting the edges in S. For an edge e of the complement of G, $G + e$ denotes the graph obtained from G by adding e.

3. Lemmas. Let H_1, H_2 be two non-trivial graphs with $u, v \in V(H_1)$, $w \in V(H_2)$. Let G_u be the graph obtained from H_1 and H_2 by identifying u with w, and G_v be the graph obtained from H_1 and H_2 by identifying v with w.

For positive integer k, let $T_i(v, k)$ ($T_i(u, k)$, respectively) be the set of closed walks of length k in G_v (G_u, respectively) starting at v (u, respectively) and an edge of H_i, and ending at an edge of H_i, where $i = 1, 2$.

LEMMA 3.1. *Suppose that* $(H_1; v) \prec (H_1; u)$. *For* $i = 1, 2$, $|T_i(v, k)| \leq |T_i(u, k)|$ *for all positive integers* k.

Proof. We only prove the case $i = 1$. The case $i = 2$ is similar.

We may decompose $W \in T_1(v, k)$ into two types of closed walks in G_v starting at v: (a) a closed walk in H_1 starting at v; (b) a closed walk in H_2 starting at v. Since $(H_1; v) \prec (H_1; u)$, we may construct an injection f_k mapping a closed walk of length k in H_1 starting at v into a closed walk of length k in H_1 starting at u.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

Now we construct a mapping f^* from $T_1(v,k)$ to $T_1(u,k)$. Let $W = W_1W_2\cdots \in T_1(v,k)$, where W_r for $r \geq 1$ is a closed walk of length l_r of type (a) if r is odd, and of type (b) if r is even. Let $f^*(W) = f^*(W_1)f^*(W_2)\cdots$, where $f^*(W_r) = f_{l_r}(W_r)$ if W_r is of type (a), and $f^*(W_r) = W_r$ if W_r is of type (b). Then $f^*(W) \in T_1(u,k)$. Obviously, f^* is an injection from $T_1(v,k)$ to $T_1(u,k)$. Then the result follows. □

A weak version of the following lemma was given by Zhang et al. [13].

Lemma 3.2. *If* $(H_1;v) \prec (H_1;u)$*, then* $EE(G_v) < EE(G_u)$.

Proof. For positive integer k, let $S_1(k)$ ($S_2(k)$, respectively) be the set of closed walks of length k in G_v (G_u, respectively) containing at least one edge of H_1 and at least one edge of H_2. Then

$$M_k(G_v) = M_k(H_1) + M_k(H_2) + |S_1(k)|,$$

$$M_k(G_u) = M_k(H_1) + M_k(H_2) + |S_2(k)|.$$

We need only to show that $|S_1(k)| \leq |S_2(k)|$ for all positive integers k, and it is strict for some positive integer k_0.

Note that

$$|S_1(k)| = |S_1^{(1)}(k)| + |S_1^{(2)}(k)|,$$

where $S_1^{(1)}(k)$ is the subset of $S_1(k)$ for which every closed walk starts at a vertex in $V(H_1)$, and $S_1^{(2)}(k)$ is the subset of $S_1(k)$ for which every closed walk starts at a vertex in $V(H_2) \setminus \{w\}$. Similarly,

$$|S_2(k)| = |S_2^{(1)}(k)| + |S_2^{(2)}(k)|,$$

where $S_2^{(1)}(k)$ is the subset of $S_2(k)$ for which every closed walk starts at a vertex in $V(H_1)$, and $S_2^{(2)}(k)$ is the subset of $S_2(k)$ for which every closed walk starts at a vertex in $V(H_2) \setminus \{w\}$.

Let $W \in S_1^{(1)}(k)$ with starting vertex x. We may uniquely decompose W into three parts, say $W_1W_2W_3$, where W_1 is a walk from x to v in H_1, W_2 is a closed walk in G_v starting at v and an edge of H_2, and ending at an edge of H_2, and W_3 is a walk from v to x in H_1. Denote by k_r the length of W_r for $r = 1,2,3$. Then $k_1, k_3 \geq 0$, $k_2 \geq 2$, and $k_1 + k_2 + k_3 = k$. Let $\mathbf{A} = \mathbf{A}(H_1)$, and let $a_{ij}^{(r)}$ be the (i,j)-entry of $\mathbf{A}^r$, which is equal to the number of walks of length r from the ith vertex to the jth vertex of H_1, see [1], where $r \geq 0$. Then

$$|S_1^{(1)}(k)| = \sum_{\substack{k_1+k_2+k_3=k \\ k_1,k_3\geq 0, k_2\geq 2}} \sum_{x\in V(H_1)} a_{xv}^{(k_1)} |T_2(v,k_2)| a_{vx}^{(k_3)}$$

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

$$= \sum_{\substack{k_1+k_2+k_3=k \\ k_1,k_3\geq 0, k_2\geq 2}} |T_2(v,k_2)| \sum_{x\in V(H_1)} a_{xv}^{(k_1)} a_{vx}^{(k_3)}$$

$$= \sum_{\substack{k_1+k_2+k_3=k \\ k_1,k_3\geq 0, k_2\geq 2}} |T_2(v,k_2)| a_{vv}^{(k_1+k_3)}.$$

Similarly,

$$|S_2^{(1)}(k)| = \sum_{\substack{k_1+k_2+k_3=k \\ k_1,k_3\geq 0, k_2\geq 2}} |T_2(u,k_2)| a_{uu}^{(k_1+k_3)}.$$

By Lemma 3.1, $|T_2(v,r)| \leq |T_2(u,r)|$ for all positive integers r. Since $(H_1;v) \prec (H_1;u)$, we have $a_{vv}^{(r)} \leq a_{uu}^{(r)}$ for all positive integers r, and it is strict for some positive integer r_0. It follows that $|S_1^{(1)}(k)| \leq |S_2^{(1)}(k)|$, and it is strict for some positive integer k_0. Similarly, $|S_1^{(2)}(k)| \leq |S_2^{(2)}(k)|$. Therefore $|S_1(k)| \leq |S_2(k)|$ for all positive integers k, and it is strict for some positive integer k_0. □

LEMMA 3.3. *Let G_1 and G_2 be connected graphs with $u \in V(G_1)$ and $v \in V(G_2)$. Let G be the graph obtained by joining $u \in V(G_1)$ with $v \in V(G_2)$ by an edge, and G' be the graph obtained by identifying $u \in V(G_1)$ with $v \in V(G_2)$, and attaching a pendant vertex to the common vertex. If $d_G(u)$, $d_G(v) \geq 2$, then $EE(G) < EE(G')$.*

Proof. Let H be the graph obtained from G by deleting the vertices in G_2 different from v. Let $k \geq 2$ be a positive integer.

For $x \in V(H)$, let $\mathcal{W}_k(H;x)$ be the set of closed walks of length k starting at x in H. Then $M_k(H;x) = |\mathcal{W}_k(H;x)|$. We construct a mapping f from $\mathcal{W}_k(H;v)$ to $\mathcal{W}_k(H;u)$. For $W \in \mathcal{W}_k(H;v)$, we may decompose W into $W = (vu)W^*(uv)$, where W^* is a closed walk of length $k-2$ starting at u in H. Let $f(W) = (uv)(vu)W^*$. Obviously, $f(W) \in \mathcal{W}_k(H;u)$ and f is an injection. Since $d_H(u) > d_H(v) = 1$, we have $M_2(H;v) < M_2(H;u)$. Thus, f is an injection but not a surjection for $k = 2$. It follows that $(H;v) \prec (H;u)$. Since G (G', respectively) can be obtained from H and G_2 by identifying $v \in V(H)$ ($u \in V(H)$, respectively) with $v \in V(G_2)$, the result follows from Lemma 3.2. □

From Eq. (2.1) and noting that $M_k(G)$ is equal to the number of closed walks of length k in G, we have immediately the following lemma [10].

LEMMA 3.4. *Let G be a connected graph and e be an edge of its complement. Then $EE(G) < EE(G+e)$.*

Let $\mathcal{G}(a,b)$ be the set of graphs obtained by attaching b pendant vertices to some vertices of K_a, where $a, b \geq 1$. For a graph G with $u, v \in V(G)$, let $r_k(G;u,v)$ be the number of walks of length k from u to v in G, and $\mathcal{W}_k(G;u,[v])$ be the set of closed walks of length k starting at u and containing v in G. Let $M_k(G;u,[v]) = |\mathcal{W}_k(G;u,[v])|$.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

LEMMA 3.5. *Let $G \in \mathcal{G}(a,b)$, where $a \geq 3$ and $b \geq 1$. Let u and v be the two distinct non-pendant vertices in G. Suppose that u has $s \geq 1$ pendant neighbors in G, and v has no pendant neighbor in G. Then $(G;v) \prec (G;u)$.*

Proof. Let k be a positive integer. Note that

$$M_k(G;v) = M_k(G-u;v) + M_k(G;v,[u]),$$

$$M_k(G;u) = M_k(G-v;u) + M_k(G;u,[v]).$$

Since $s \geq 1$, $G-u$ is a proper subgraph of $G-v$, and thus $(G-u;v) \prec (G-v;u)$. We need only to show that $M_k(G;v,[u]) \leq M_k(G;u,[v])$.

For $W \in \mathcal{W}_k(G;v,[u])$, we may decompose W into two parts, say W_1W_2, where W_1 is the shortest (v,u)-section in W, and W_2 is the remaining (u,v)-section of W. Denote by $w_1, w_2, \ldots, w_{a-2}$ the common neighbors of u and v in G. Let H be the graph obtained from G by deleting the s pendant neighbors of u in G. By the choice of W_1, we know that W_1 consists of a closed walk starting at v in $H-u$ whose length may be zero and a single edge vu, or a walk from v to w_i in $H-u$ and a single edge w_iu for $1 \leq i \leq a-2$. Note that $r_k(G;u,v) = r_k(G;v,u)$ [1]. Then

$$M_k(G;v,[u]) = \sum_{\substack{x \in \{v,w_1,w_2,\ldots,w_{a-2}\} \\ k_1+k_2=k \\ k_1,k_2 \geq 1}} r_{k_1-1}(H-u;v,x)r_{k_2}(G;u,v).$$

Similarly,

$$\begin{aligned} M_k(G;u,[v]) &= \sum_{\substack{x \in \{u,w_1,w_2,\ldots,w_{a-2}\} \\ k_1+k_2=k \\ k_1,k_2 \geq 1}} r_{k_1-1}(G-v;u,x)r_{k_2}(G;v,u) \\ &\geq \sum_{\substack{x \in \{u,w_1,w_2,\ldots,w_{a-2}\} \\ k_1+k_2=k \\ k_1,k_2 \geq 1}} r_{k_1-1}(H-v;u,x)r_{k_2}(G;u,v). \end{aligned}$$

Note that $H-u \cong H-v$. For positive integer s, $r_s(H-u;v,v) = r_s(H-v;u,u)$, and $r_s(H-u;v,x) = r_s(H-v;u,x)$ if $x \in \{w_1, w_2, \ldots, w_{a-2}\}$. Therefore $M_k(G;v,[u]) \leq M_k(G;u,[v])$. ∎

LEMMA 3.6. *Let $G \in \mathcal{G}(a,b)$, where $a \geq 3$ and $b \geq 2$. If $G \ncong G_{a+b,b}$, then $EE(G) < EE(G_{a+b,b})$.*

Proof. Since $G \ncong G_{a+b,b}$, we may choose two non-pendant vertices, say u and v, such that both u and v have at least one pendant neighbor in G. Suppose that v has $t \geq 1$ pendant neighbors. Let H be the graph obtained from G by deleting the t pendant neighbors of v.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

Let G_1 be the graph obtained from H and the star S_{t+1} on $t+1$ vertices by identifying u with the center of S_{t+1}. Note that G can be obtained from H and the star S_{t+1} by identifying v with the center of S_{t+1}. By Lemma 3.5, $(H; v) \prec (H; u)$. Then $EE(G) < EE(G_1)$ follows from Lemma 3.2. Repeating the transformation from G to G_1, we may finally have $EE(G) < EE(G_{a+b,b})$. □

4. Main result. Now we prove our main result.

THEOREM 4.1. *Let* $G \in \mathbb{G}(n, r)$*, where* $0 \le r \le n-3$*. Then* $EE(G) \le EE(G_{n,r})$ *with equality if and only if* $G \cong G_{n,r}$*.*

Proof. The case $r = 0$ follows from Lemma 3.4.

Suppose that $r \ge 1$. Let G be a graph in $\mathbb{G}(n, r)$ with maximum Estrada index. Let S be the set of cut edges in G. Obviously, $G - S$ consists of $r + 1$ connected components. By Lemma 3.4, all these connected components are complete.

If there exists some edge, say u_1v_1, of S such that $d_G(u_1)$, $d_G(v_1) \ge 2$, then applying Lemma 3.3 to G by setting $u = u_1$ and $v = v_1$, we may get a graph in $\mathbb{G}(n, r)$ with a larger Estrada index, a contradiction. Thus, every cut edge of G has exactly one end vertex with degree one, i.e., every cut edge of G is incident to a pendant vertex. Then G is a graph obtained by attaching r pendant vertices to some vertices of K_{n-r}, i.e., $G \in \mathcal{G}(n - r, r)$.

If $r = 1$, then obviously $G \cong G_{n,1}$. If $2 \le r \le n - 3$, then by Lemma 3.6, we have $G \cong G_{n,r}$. □

REFERENCES

[1] D. Cvetković, M. Doob, and H. Sachs. *Spectra of Graphs – Theory and Application*. Academic Press, Inc., New York, 1980.

[2] J.A. de la Peña, I. Gutman, and J. Rada. Estimating the Estrada index. *Linear Algebra and its Applications*, 427:70–76, 2007.

[3] H. Deng. A proof of a conjecture on the Estrada index. *MATCH Communications in Mathematical and in Computer Chemistry*, 62:599–606, 2009.

[4] E. Estrada. Characterization of 3D molecular structure. *Chemical Physics Letters*, 319:713–718, 2000.

[5] E. Estrada. Characterization of the folding degree of proteins. *Bioinformatics*, 18:697–704, 2002.

[6] E. Estrada. Characterization of the amino-acids contribution to the folding degree of proteins. *Proteins: Structure, Function and Bioinformatics*, 54:727–737, 2004.

[7] E. Estrada and J.A. Rodríguez–Valázquez. Subgraph centrality in complex networks. *Physical Review E. Statistical, Nonlinear, and Soft Matter Physics*, 71:056103, 9 pages, 2005.

[8] E. Estrada and J.A. Rodríguez–Valázquez. Spectral measures of bipartivity in complex networks. *Physical Review E. Statistical, Nonlinear, and Soft Matter Physics*, 72:046105, 6 pages, 2005.

Electronic Journal of Linear Algebra ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 22, pp. 586-592, June 2011

ELA
http://math.technion.ac.il/iic/ela

[9] E. Estrada, J.A. Rodríguez–Valázquez, and M. Randić. Atomic branching in molecules. *International Jounal of Quantum Chemistry*, 106:823–832, 2006.

[10] I. Gutman, E. Estrada, and J.A. Rodríguez–Velázquez. On a graph–spectrum–based structure descriptor. *Croatica Chemica Acta*, 80:151–154, 2007.

[11] A. Ilić and D. Stevanović. The Estrada index of chemical trees. *Journal of Mathematical Chemistry*, 47:305–314, 2010.

[12] H. Liu, M. Lu, and F. Tian. On the spectral radius of graphs with cut edges. *Linear Algebra and its Applications*, 389:139–145, 2004.

[13] J. Zhang, B. Zhou, and J. Li. On Estrada index of trees. *Linear Algebra and its Applications*, 434:215–223, 2011.

[14] B. Zhou. On Estrada index. *MATCH Communications in Mathematical and in Computer Chemistry*, 60:485–492, 2008.

[15] B. Zhou and N. Trinajstić. Estrada index of bipartite graphs. *International Journal of Chemical Modeling*, 1:387–394, 2008.