International Journal of Mathematics and Statistics Invention (IJMSI)
E-ISSN: 2321 – 4767 P-ISSN: 2321 - 4759
www.ijmsi.org Volume 4 Issue 6 || August. 2016 || PP-35-38

The Fourth Largest Estrada Indices for Trees

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ABSTRACT
Let G be a simple graph with n vertices, and $\lambda_1, \cdots, \lambda_n$ *be the eigenvalues of its adjacent matrix. The Estrada index of G is a graph invariant, defined as* $EE = \sum_{i=1}^{n} e^{\lambda_i}$ *,, is proposed as a measure of branching in alkanes. In this paper, we obtain two candidates which have the fourth largest EE among trees with n vertices.*

Keywords: *Estrada index; trees; extremal graph*

I. Introduction

Throughout the paper, G is a simple graph with vertex set $V = \{v_1; ...; v_n\}$ and the edge set E. Let $A(G)$ be the adjacent matrix of G, which is a symmetric (0; 1) matrix. The spectrum of G is the eigenvalues of its adjacency matrix, which are denoted by $\lambda_1, \cdots, \lambda_n$. For basic properties of graph eigenvalues, the readers are referred to [1]. A graph-spectrum-based invariant, put forward by Estrada [2], is defined as

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

EE is usually referred as the Estrada index. The Esteada index has been successfully related to chemical properties of organic molecules, especially proteins[2-3]. Estrada and Rodriguez-Velazquez[4-5] showed that *EE* provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. It was also proposed as a measure of molecular branching[6]. Within groups of isomers, *EE* was found to increase with the increasing extent of branching of carbon-atom skeleton. In addition, EE characterizes the structure of alkanes via electronic partition function. Therefore it is natural to investigate the relations between the Estrada index and the graph-theoretic properties of G. Let $d(u)$ denote the degree of vertex u. A vertex of degree 1 is called a pendant vertex or a leaf. A connected graph without any cycle is a tree. The path P_n is a tree of order n with exactly two pendant vertices. The star of order n, denoted by Sn is a tree with $n - 1$ pendant vertices. Let $d(u)$ denote the degree of vertex u. A vertex of degree 1 is called a pendant vertex. A connected graph without any cycle is a tree. The path Pn is a tree of order n with exactly two pendant vertices. The star of order n, denoted by S_n, is a tree with $n - 1$ pendant vertices. The double star of order n, denoted by $S(p, q)$, is a tree with $n - 2$ pendant vertices. p, q are the degrees of vertices whose degrees are bigger than 1 in $S(p, q)$ The $\Delta-$starlike $T(n_1, ..., n_\Delta)$ is a tree composed of the root v, and the paths $P_1, P_2, ...,$ $P\Delta$ of length $n_1, n_2, ..., n_\Delta$ attached at v. The number of vertices of a tree $T(n_1, ..., n_\Delta)$ equals $n = n_1 + n_2 + ... + n_\Delta$.

A walk in a graph G is a finite non-null sequence $w = v_0e_1v_1e_2v_2{\dots}v_{k-1}e_kv_k$, whose terms are alternately vertices and edges, such that, for every $1 \le i \le k,$ the ends of e_i are v_{i-1} and v_i. We say that w is a walk from v_0 to v_k, or a $(v_0, v_k)-$ walk. The vertices v_0 and v_k are called the initial and final vertices of w, respectively, and $v_1, ..., v_{k-1}$ its internal vertices. The integer k is the length of w. The walk is closed if $v_0 = v_k$.

In a simple graph, a walk $v_1e_1v_2e_2v_3\ldots v_{k-1}e_{k-1}vk$ is determined by the sequence $v_1v_2...v_{k-1}v_k$ of its vertices, hence a walk in a simple graph can be simply specified by its vertex sequence.

For any vertex u in G, we denote by $S_k(G, u)$ the set of walks in G with length k starting from u, and by $M_k(G, u)$ the number of walks in G with length k starting from u. Therefore, the set of all closed walks of length k in G, denoted by $S_k(G)$, equals to $\bigcup_{v\in G} S_k(G, v)$, and $M_k(G) = \sum_{v\in G} M_k(G, v)$ **Error! Reference source not found.**. The diameter of G, denoted by $Diam(G)$ is the length of the longest path in G. Since every tree is a bipartite graph, there is no any self-returning walk with odd length in a tree.

For the path $P_n = v_1v_2...v_n$ and the star S_n with center v_1, and any integer $k \geq 0$, we have $M_k(P_n, v_i) = M_k(P_n, v_{n-i+1})$ and $M_k(S_n, v_j) = M_k(S_n, v_t)$ for all $1 \leq i \leq n$ and $2 \leq j, t \leq n$ by symmetry.

Some mathematical properties of the Estrada index were established. One of most important properties is the following:

$$EE=\sum_{k\geqslant 0}(M_k(G))/k!$$

$M_k(G)$ is called the k-th spectral moment of the graph G. $M_k(G)$ is equal to the number of closed walks of length k in G. Thus, if for two graphs G_1 and G_2, we have $M_k(G_1) \geqslant M_k(G_2)$ for all $k \geqslant 0$, then $EE(G_1)\geqslant EE(G_2)$. Moreover, if there is at least one positive integer t such that $M_t(G_1) > M_t(G_2)$, then $EE(G_1) > EE(G_2)$. The question of finding the lower and upper bounds for EE and the corresponding extremal graphs attracted the attention of many researchers.G, J. A. de la Penna, I. Gutman and J. Rada [9] established lower and upper bounds for EE in terms of the number of vertices and number of edges and some inequalities between EE and the energy of G. Deng showed that among n-vertex trees, P_n has the minimum and Sn the maximum Estrada index, and among connected graphs of order n, the path P_n has the minimum Estrada index. Among these, Ilic and Stevanovic[10] obtained the unique tree with minimum Estrada index among the set of trees with given maximum degree, and determines the tree with second minima EE. Zhang et al. [11] determined the unique tree with maximum Estrada index among the set of trees with given matching number. Zhang et al.[11] determined the unique tree with maximum Estrada index among the set of trees with given matching number. In [12], Li proved that, among trees with n vertices, $S(2; n - 2)$ and $S(3; n - 3)$ have the second and the third largest EE, respectively. In this paper, we obtain two candidates which have the fourth largest EE among trees with n vertices.

II. Main results

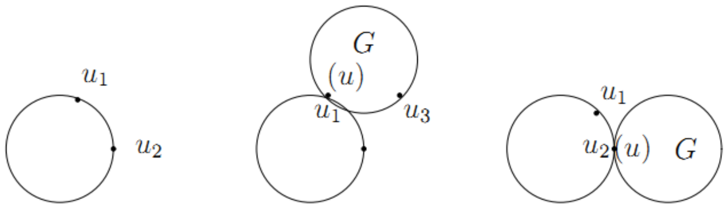
First of all, we list and prove some lemmas, which will be used later.

Lemma 2.1[12] Let $G = S(p, q)$ be a double star with centers w, v and leaves u_i, $i = 1, 2, ..., p+q$-2, and assume that $d(w) = p$ and $d(v) = q$. Then $M_k(G, v) > M_k(G, u_i)$ and $M_k(G, w) > M_k(G, u_i)$ for all $i = 1, 2, ..., p + q-2$. If $p \leq q$, then $M_k(G, w) \leq M_k(G, v)$ for every $k \geq 1$, and $M_k(G, w) < M_k(G, v)$ for at least one integer k_0 if $p < q$.

Lemma 2.2[10] Let $P_n = v_1v_2...v_n$. For every $k \geq 0$, the following hold: $M_k(P_n, v_1) \leq M_k(P_n, v_2) \leq ... \leq M_k(P_n, v$**Error! Reference source not found.**$_{n/2})$ with strict inequality for sufficiently large k.

Lemma 2.3[12] Let v be a pendant vertex of a simple graph G, and v_1 is the only vertex connecting v. We have an injection η_k from $S_k(G, v)$ to $S_k(G, v_1)$ for every $k \geq 1$, and η_{k0} is not surjective for at least one integer k_0 if v_1 is an internal vertex. Therefore, $M_k(G, v) \leq M_k(G, v_1)$ for every $k \geq 1$, and $M_{k0}(G, v) < M_{k0}(G, v_1)$ for at least one integer k_0.

Lemma 2.4[12] Let u_1, u_2 be two non-isolated vertices of a simple graph H , u be a non-isolated vertices of a simple graph G. If H_1 and H_2 are the graphs obtained from H by identifying u_1 and u_2 to u, respectively, depicted in Figure 1. If $M_k(H, u_1) \leq M_k(H, u_2)$ for all integer $k \geq 0$, and $M_{k0}(H, u_1) < M_{k0}(H, u_2)$ for at least one integer k_0, then $M_t(H_1) \leq M_t(H_2)$ for all integer $t \geq 0$,and $M_{t0}(H_1) < M_{t0}(H_2)$ for at least one integer t_0.



H H_1 H_2

Fig. 1

For $n = 5$, we only have three trees: S_5, P_5, $P_{5,3}$. Therefore, we only need consider $n > 5$ in the following.

Lemma 2.5 If G has the fourth largest Estrada index among trees with n vertices, then Diam(G)<5.

Proof Let G be a tree with fourth maximal Estrada index. On the contrary, we assume that $Diam(T) \geq 5$. Let $T = v_1v_2...v_k$ be the longest path in G, and let $v_{k+1}, ..., v_{d-2}$ are neighbours of v_2 besides v_1 and v_3, where d is the degree of v_2. By cutting v_1v_2, $v_{k+1}v_2$, ..., $v_{d-2}v_2$ and adding new edges v_1v_3, $v_{k+1}v_3$, ..., $v_{d-2}v_3$, we get a new tree G_1 of order n. $G_1 \neq S_n$ because $Diam(G_1) \geq 4$.

On the other hand, we can obtain G and G_1 by identifying the center u of $Gd-1$ to v_2 and v_3 of $G - \{v_1, v_k, ..., v_{d-2}\}$, respectively. By lemma 2.2, $M_k(G_2, v_2) \leq M_k(G_2, v_3)$ for every $k \geq 1$. Therefore, $M_k(G) \leq M_k(G_1)$ for all integer $k \geq 0$, and $Mk_0\ (G) < Mk_0\ (G_1)$ for at least one integer k_0 by lemma 2.4. Thus $EE(G) < EE(G_2)$ by equation (2). We get a tree G_1 with bigger EE than G, a contradiction. Hence $Diam(G) \leq 4$..

Proposition 2.1[12] Among trees with $k \geq 6$ vertices, the double star $S(3, n - 3)$ has the third largest Estrada index.

Theorem 2.1 If $n = 6$, 3-starlike tree $T(2, 2, 1)$ has the fourth largest Estrada index; If $n = 7$, 4-starlike tree $T(2, 2, 1, 1)$ has the fourth largest Estrada index. For $n \geq 8$, $S(4, n - 4)$ or n-3−starlike tree $T(2, 2, 1, 1, ..., 1)$ has the fourth largest Estrada index.

Proof For $n = 6$, If we only have two double star trees $S(2, 4)$ and $S(3, 3)$. By Lemma 2.5, if G has the fourth largest Estrada index, then $Diam(G) = 4$. We just need to add a pendent edge at one of internal vertex of the path P_4. By lemma 2.2 and lemma 2.4, $EE(T(2, 2, 1)) > EE(T(3, 1, 1))$. So, $T(2, 2, 1)$ has the fourth largest Estrada index.

For $n = 7$, we only have two double star trees: $S(2, 5)$ and $S(3, 4)$. By Lemma 2.5, if G has the fourth largest Estrada index, then $Diam(G) = 4$. We just need to add a pendent path of length 2 at v_3 of the path $P_4 = v_1v_2v_3v_4v_5$ or add two pendent edges at two of internal vertex of the path P_4. If $v_3v_6v_7$ is a pendant path attached at v_3, we can cut the edge v_6v_7 and add a new edge v_7v_3 to form a new tree with bigger Estrada index by Lemma 2.2 and lemma 2.4. So, $T(3, 3, 3)$ is not the tree with fourth largest Estrada index. In the same way, we can show that $T(2, 2, 1, 1)$ has the fourth largest Estrada index.

For $n \geq 8$, let $P = v_1v_2v_3v_4v_5$ be the longest path in T. If v_2 or v_4 has a pendent path of length longer than 1, we can choose another path with length bigger than 5, a contradiction. In the same way, we can prove that all pendent path at v_3 have the length shorter than 2. If $v_3v_6v_7$ is a pendant path attached at v_3, we can cut the edge v_6v_7 and add a new edge v_7v_3 to form a new tree with bigger Estrada index by Lemma 2.1 and lemma 2.2. So, all pendant paths at v_3, v_4 and v_5 are of length 1.

If $d(v_2) > 2$ and $d(v_4) > 2$, we cut v_4w_1, ..., v_4wt and add new edges v_3w_1, ..., v_3wt to form a new tree T_1. Obviously, $T_1 \neq S(3, n - 3)$. By lemma 2.1 and lemma 2.2, $EE(T_1) > EE(T)$, a contradiction.

Without loss of generality, we assume that $d(v_4) = 4$. We will compare the Estrada index of the following three kinds of trees T_2, $T_3 = T(2, 2, 1, ..., 1)$, $T_4 = T(3, 1, 1, ..., 1)$, as shown in Figure 2.

Fig.2

We can obtain T_2 from T_5 by adding some new edges w_1v_3, ..., wtv_3. Also We can obtain T_3 from T_5 by adding some new edges w_1v_3, ..., wtv_3. By lemma 3.2, $S_k(P_5, v_3) \geq S_k(P_5, v_2)$ for all k and $Sk_0\ (P_5, v_3) > Sk_0\ (P_5, v_2)$ for at least one integer k_0. Then $S_k(T_5, v_3) \geq S_k(T_5, v_2)$ by lemma 3.1. Therefore, $EE(T_3) > EE(T_2)$.

By lemma 2.2, $EE(T_3) > EE(T_4)$ since $M_k(P_5, v_3) \geq M_k(P_5, v_2)$ and $M_{k1}\ (P_5, v_3) \geq M_{k1}\ (P_5, v_2)$for at least one integer k_1. From above discussion, T_3 has the largest Estrada index among $n-$vertex trees with length 4. If a graph G has diameter 3, then G is a double star. By lemma 2.1, $EE(S(2, n\text{-}2)) > EE(S(3, n-3)) > EE(S(4, n-4))$ .For $n \geq 8$, Trees with fourth largest trees may be T_3 or $S(4, n-4)$.

Acknowledgement

The project was supported by Hunan Provincial Natural Science Foundation of China(13JJ4103) and The Education Department of Hunan Province Youth Project(12B067).

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