MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **61** (2009) 495-501

ISSN 0340 - 6253

On the Estrada Index of Bipartite Graph[1]

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(Received May 5, 2008)

Abstract

For a graph G of n vertices, let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of its adjacency matrix. The Estrada index of G is defined by $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. In this paper, we give some new lower and upper bounds for EE of bipartite graphs. We determine the first three trees with the greatest Estrada index.

1 Introduction

All graphs considered here are finite and simple. Notations and terminology not defined will conform to those in [2]. For a graph G, let n and m denote the number of vertices and the number of edges, respectively. A (n, m)–graph means a graph with n vertices and m edges. For a graph G, its characteristic polynomial $P(G, x)$ is the characteristic polynomial of its adjacency matrix, that is, $P(G, x) = det(xI - A(G))$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of its adjacency matrix $A(G)$. Then the spectrum of G is $Spec(G) = \{\lambda_1, \lambda_2, \cdots, \lambda_n\}$. The number of zero eigenvalues in the spectrum of the graph G is called its nullity and is denoted by $\eta(G)$, see [17].

A graph-spectrum-based graph invariant, recently put forward by Estrada [3-7], is defined as

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

EE is nowadays usually referred to as the Estrada index, see [9-12,15].

Although invented only a few years ago [3, 4], the Estrada index has already found numerous applications. It was used to quantify the degree of folding of long-chain molecules, especially proteins [3–5]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE was put forward by Estrada and Rodríguez-Velázquez [6, 7]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. In addition to this, in a recent work [8] a connection

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between EE and the concept of extended atomic branching was considered. Very recently the authors in [11, 12, 13, 16] established some lower and upper bounds for EE and gave some general mathematical properties of the Estrada index. In particular, from [3-16] we found the following results:

1. [7] Denoting by $M_k = M_k(G) = \sum\limits_{i=1}^{n} {\lambda_i}^k$ the kth spectral moment of the graph G, then

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

2. [8] For a bipartite graph G, if $\eta(G)$ is the multiplicity of its eigenvalue zero, then

$$EE(G) = \eta(G) + 2\sum_{+} ch(\lambda_i), \tag{1}$$

where $ch(x) = \frac{e^x+e^{-x}}{2}$, $\sum\limits_{+}$ denotes the summation over all positive eigenvalues of the corresponding graph.

3. [16] For a (n, m)–graph G, the Estrada index of G is bounded by

$$\sqrt{n^2+4m} \leq EE(G) \leq n - 1 + e^{\sqrt{2m}}, \tag{2}$$

where the equality of both sides holds if and only if $G \cong \overline{K_n}$.

4. [16] For a bipartite (n, m)–graph G, the Estrada index of G is bounded by

$$\sqrt{n^2+4m} \leq EE(G) \leq n - 2 + ch(\sqrt{m}), \tag{3}$$

where the equality of lift-hand side of (3) holds if and only if $G \cong \overline{K_n}$ and the equality of right-hand side of (3) is attained for graphs of form $G \cong K_{a,b} \cup \overline{K_c}$, with $a, b, c \geq 0$, $a + b + c = n$ and $ab = m$.

Very recently, Gutman in [13] gave some lower bounds of Estrada index of a graph as follows:

5. If G is an (n, m)-graph with at least one edge and nullity $\eta(G) > 0$, then

$$EE(G) \geq \eta(G) + (n - \eta(G))ch\left(\sqrt{\frac{2m}{n-\eta(G)}}\right).$$

Equality holds if and only if G consists either of isolated vertices and copies of K_2, or of isolated vertices and copies of various complete bipartite graphs $K_{a,b}$ with the product $a \cdot b$ is constant.

The authors in [16] posed the following conjecture.

Conjecture A. Among n-vertex trees, the path has minimum and the star maximum Estrada index, that is,

$$EE(S_n) > EE(T_n) > EE(P_n),$$

where T_n is a tree of n vertices and $T_n \notin \{S_n, P_n\}$.

In this paper, our main goal is to investigate the Estrada index of bipartite graphs. Some new lower and upper bounds for EE of bipartite graphs are obtained. We determine the first three trees with the greatest Estrada index, thus proving the first inequality of Conjecture A.

2 Some Lemmas

In this section, at first we consider the following function.

$$f_k(x_1, x_2, \cdots, x_t) = x_1^k + x_2^k + \cdots + x_t^k, \tag{4}$$

where k is a positive integer, $x_1 \geq x_2 \geq x_3 \cdots \geq x_t \geq 0$ and $\sum_{i=1}^{t} x_i = m$.

Lemma 1. If $x_i - x_j \geq 2\alpha > 0$ for some i and j, then for $k \geq 2$ we have

$$f_k(x_1, x_2, \cdots, x_i, \cdots, x_j, \cdots, x_t) > f_k(x_1, x_2, \cdots, x_i - \alpha, \cdots, x_j + \alpha, \cdots, x_t).$$

Proof. Note that

$$\begin{aligned} & f_k(x_1, x_2, \cdots, x_i, \cdots, x_j, \cdots, x_t) - f_k(x_1, x_2, \cdots, x_i - \alpha, \cdots, x_j + \alpha, \cdots, x_t) \\ & = x_i^k - (x_i - \alpha)^k + x_j^k - (x_j + \alpha)^k \\ & = \alpha \sum_{r=1}^{k} \left(x_i^{k-r}(x_i - \alpha)^{r-1} - x_j^{k-r}(x_j + \alpha)^{r-1} \right). \end{aligned}$$

By $x_i - x_j \geq 2\alpha > 0$, the result follows. □

By Lemma 1, it is easy to get that

Lemma 2. For $k \geq 2$,

$$\frac{m^k}{t^{k-1}} \leq f_k(x_1, x_2, \cdots, x_t) \leq m^k, \tag{5}$$

where the equality of lift-hand side of (5) holds if and only if $x_i = \frac{m}{t}$ for all i, while the equality of right-hand side of (5) holds if and only if $x_1 = m$ and $x_i = 0$ for $i \geq 2$. □

3 Estrada index of bipartite graph

It is easy to see that if G has k connected components $G_1, G_2, \cdots, G_k$, then $EE(G) = \sum_{i=1}^{k} EE(G_i)$. So, we shall investigate the Estrada index of connected bipartite graph here. From Theorem 2 in [13] and Theorem 5 in [16], one find the following result. By Lemmas 1 and 2 we give a new proof of the result.

Theorem 1([13, 16]). For a connected bipartite (n, m)–graph G with $n \geq 2$, the Estrada index of G is bounded by

$$\eta(G) + (n - \eta(G))ch\left(\sqrt{\frac{2m}{n - \eta(G)}}\right) \leq EE(G) \leq n - 2 + 2ch(\sqrt{m}), \tag{6}$$

where the equality of left-hand side of (6) holds if and only if all positive eigenvalues are equal, while the equality of right-hand side of (6) holds if and only if G is a complete bipartite graph.

Proof. Let G be a connected bipartite graph, by (1) we have

$$\begin{aligned} EE(G) &= \eta(G) + 2\sum_{+} \sum_{k=0}^{\infty} \frac{\lambda_i^{2k}}{(2k)!} \\ &= \eta(G) + 2\sum_{k=0}^{\infty} \frac{1}{(2k)!} \sum_{+} \lambda_i^{2k}. \end{aligned}$$

It is well known that the eigenvalues of bipartite graphs are symmetric respect to zero. Then G has $t = (n - \eta(G))/2$ positive eigenvalues and $\sum_{+} \lambda_i^2 = m$. Set $x_i = \lambda_i^2$ for $1 \leq i \leq t$. By Lemma 2, for all $k \geq 2$ we have that $\sum_{+} \lambda_i^{2k}$ attains the minimum value if and only if all positive eigenvalues are equal and attains the maximum value if and only if G has only one positive eigenvalue, that is, $t = 1$. Note that a connected bipartite G has only one positive eigenvalue if and only if G is a complete bipartite graph, see [17]. Therefore, the results follows from (1). □

As a corollary of Theorem 1, we have

Corollary 1. The star n has maximum Estrada index among all trees of n vertices, that is

$$EE(S_n) > EE(T_n),$$

where T_n is a tree of n vertices and $T_n \ncong S_n$. □

Let $\lambda_1(G)$ be the greatest eigenvalue of G. Then, $\sum_{+,i\geq 2} \lambda_i^2 = m - \lambda_1(G)^2$, where $\sum_{+,i\geq 2}$ denotes the summation over all positive eigenvalues except for $\lambda_1(G)$. A proof similar with that of Theorem 1, one show that

Theorem 2. For a connected bipartite (n, m)–graph G, the Estrada index of G is bounded by

$$\begin{aligned} &\eta(G) + ch\left(\sqrt{m - \lambda_1^2(G)}\right) + (n - \eta(G) - 2)ch\left(\sqrt{\tfrac{2m}{n-\eta(G)-2}}\right) \\ &\leq EE(G) \leq n - 4 + ch(\lambda_1(G)) + ch\left(\sqrt{m - \lambda_1^2(G)}\right), \end{aligned} \tag{7}$$

where the equality of left-hand side of (7) holds if and only if all positive eigenvalues except for $\lambda_1(G)$ are equal, while the equality of right-hand side of (7) holds if and only if G has four nonzero eigenvalues. □

4 Trees with the maximal Estrada indices

For a tree T with n vertices, from [17] one find that if the order of the maximum matching is θ, then $\eta(T) = n - 2\theta$, that is, T has θ positive eigenvalues. By Theorem 1, we have

Theorem 3. Let T a tree of n $(n \geq 2)$ vertices with the order θ of the maximum matching. Then its Estrada index is bounded by

$$n - 2\theta + \theta ch\left(\sqrt{\frac{2(n-1)}{\theta}}\right) \leq EE(T) \leq n - 2 + 2ch(\sqrt{n-1}), \tag{8}$$

where the equality of left-hand side of (8) holds if and only if all positive eigenvalues are equal, while the equality of right-hand side of (8) holds if and only if $G \cong S_n$.□

Theorem 4. Let T_1 and T_2 be two trees of n vertices. If T_1 has exactly two positive eigenvalues and T_2 has at least two positive eigenvalues with $\lambda_1(T_1) > \lambda_1(T_2)$, then $EE(T_1) > EE(T_2)$.

Proof. Let $\lambda_1(T_1)$ and $\lambda_2(T_1)$ be two positive eigenvalues of T_1. Denote by

$\lambda_1(T_2), \lambda_2(T_2), \cdots, \lambda_t(T_2)$ all positive eigenvalues of T_2 with $\lambda_1(T_2) \geq \lambda_2(T_2) \geq \cdots \geq \lambda_t(T_2)$. By (1), it follows that

$$EE(T_1) = n - 4 + 2\sum_{k=0}^{\infty} \frac{1}{(2k)!} f_k(\lambda_1^2(T_1), \lambda_2^2(T_1)), \tag{9}$$

$$EE(T_2) = \eta(T) + 2\sum_{k=0}^{\infty} \frac{1}{(2k)!} f_k(\lambda_1^2(T_2), \lambda_2^2(T_2), \cdots, \lambda_t^2(T_2)), \tag{10}$$

where $\lambda_1^2(T_1) + \lambda_2^2(T_1) = \lambda_1^2(T_2) + \lambda_2^2(T_2) + \cdots + \lambda_t^2(T_2) = n - 1$.

Since $\lambda_1(T_1) > \lambda_1(T_2)$, by Lemma 1, we have

$$f_k(\lambda_1^2(T_1), \lambda_2^2(T_1)) > f_k(\lambda_1^2(T_2), \lambda_2^2(T_2), \cdots, \lambda_t^2(T_2)),$$

for $k \geq 2$. By (9) and (10), $EE(T_1) > EE(T_2)$. $\square$

The authors in [14] determine the first six trees with the greatest eigenvalue, see Figure 1, where S_n^i is the tree with the ith greatest eigenvalue.

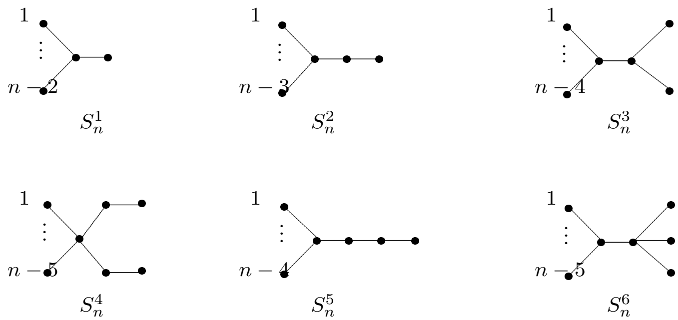

Figure 1. Trees $S_n^i, i = 1, 2, 3, 4, 5, 6$

From [14], $\lambda_1(S_n^1) > \lambda_1(S_n^2) > \lambda_1(S_n^3) > \lambda_1(S_n^4) > \lambda_1(S_n^5) > \lambda_1(S_n^6)$, for $n \geq 5$. By direct computation, one see that S_n^i, for $i = 2, 3, 4, 6$, have exactly two positive eigenvalues. So, by Theorems 1 and 4, for two trees T_n^1 and T_n^2 of $n \geq 5$ vertices we have

$$EE(S_n^1) > EE(S_n^2) > EE(S_n^3) > EE(S_n^5) > EE(S_n^6) > EE(T_n^1)$$

and

$$EE(S_n^1) > EE(S_n^2) > EE(S_n^3) > EE(T_n^2),$$

where $T_n^1 \notin \{S_n^i | i = 1, 2, 3, 4, 5, 6\}$ and $T_n^2 \notin \{S_n^i | i = 1, 2, 3\}$. Therefore we have

Theorem 5. Among trees of n vertices, the first three trees with the greatest Estrads index are S_n^1, S_n^2 and S_n^3, respectively. $\square$

5 Remarks

Let $n \geq 6$, by direct computation, for S_n^4 and S_n^5 we have

$$EE(S_n^4) = n - 6 + e^{\sqrt{-1+n/2+1/2\sqrt{24-8n+n^2}}} + e^{-\sqrt{-1+n/2+1/2\sqrt{24-8n+n^2}}} + e^{\sqrt{-1+n/2-1/2\sqrt{24-8n+n^2}}} + e^{-\sqrt{-1+n/2-1/2\sqrt{24-8n+n^2}}} + e + e^{-1},$$

$$EE(S_n^5) = n - 4 + e^{\sqrt{-1/2+n/2+1/2\sqrt{29-10n+n^2}}} + e^{-\sqrt{-1/2+n/2+1/2\sqrt{29-10n+n^2}}} + e^{\sqrt{-1/2+n/2-1/2\sqrt{29-10n+n^2}}} + e^{-\sqrt{-1/2+n/2-1/2\sqrt{29-10n+n^2}}}.$$

Using software Mathematics, by calculating we find $EE(S_n^4) > EE(S_n^5)$ for $n \geq 6$. It is not easy to prove that $EE(S_n^4) > EE(S_n^5)$. Therefore, we shall try to find some new methods to prove it and to determine the first thirteen trees with the greatest Estrada index by using the results in [1, 15].

Acknowledgements

We would like to express our thanks to the referees for the valuable comments and Professor Gutman for sending his paper in press.

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