On maximum Estrada indices of bipartite graphs with some given parameters*

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Abstract

The Estrada index of a graph G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where λ_1, $\lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. In this paper, we characterize the unique bipartite graph with maximum Estrada index among bipartite graphs with given matching number and given vertex-connectivity, edge-connectivity, respectively.

Keywords: Estrada index; walk; maximum matching; vertex cut; connectivity

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1 Introduction

Let G be a simple graph on n vertices. The eigenvalues of G are the eigenvalues of its adjacency matrix, which are denoted by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. The Estrada index of G, put forward by Estrada [7], is defined as

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

The Estrada index has multiple applications in a large variety of problems, for example, it has been successfully employed to quantify the degree of folding of long-chain molecules,

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especially proteins [8, 9, 10], and it is a useful tool to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks [11, 12]. There is also a connection between the Estrada index and the extended atomic branching of molecules [13]. Besides these applications, the Estrada index has also been extensively studied in mathematics, see [16, 18, 20, 21, 22]. Ilić and Stevanović [16] obtained the unique tree with minimum Estrada index among the set of trees with a given maximum degree. Zhang, Zhou and Li [20] determined the unique tree with maximum Estrada indices among the set of trees with a given matching number. In [4], Du and Zhou characterized the unique unicyclic graph with maximum Estrada index. Wang et al. [19] determined the unique graph with maximum Estrada index among bicyclic graphs with fixed order, and Zhu et al. [23] determined the unique graph with maximum Estrada index among tricyclic graphs with fixed order. More mathematical properties on the Estrada index can be founded in [14].

A graph is bipartite if its vertex set can be partitioned into two subsets X and Y so that every edge has one end in X and the other end in Y. We denote a bipartite graph G with bipartition (X, Y) by $G[X, Y]$. If $G[X, Y]$ is simple and every vertex in X is joined to every vertex in Y, then G is called a complete bipartite graph. Up to isomorphism, there is a unique complete bipartite graph with parts of sizes m and n, denoted $K_{m,n}$. For an edge subset A of the complement of G, we use $G+A$ to denote the graph obtained from G by adding the edges in A.

A matching in a graph is a set of pairwise nonadjacent edges. If M is a matching, the two ends of each edge of M are said to be matched under M, and each vertex incident with an edge of M is said to be covered by M. A maximum matching is one which covers as many vertices as possible. The number of edges in a maximum matching of a graph G is called the matching number of G and denoted by $\alpha'(G)$. Let $\mathcal{M}_{n,p}$ be the set of bipartite graphs on n vertices with $\alpha'(G) = p$.

A cut vertex(edge) of a graph is a vertex(edge) whose removal increases the number of components of the graph. A(An) vertex(edge) cut of a graph is a set of vertices(edges) whose removal disconnects the graph. The connectivity(edge-connectivity) of a graph G is defined as

$$\kappa(G) = \min\{|S| : S \text{ is a vertex cut of } G\}, \kappa'(G) = \min\{|S| : S \text{ is an edge cut of } G\}.$$

Let $\mathcal{C}_{n,s}(\mathcal{D}_{n,s})$ denote the set of bipartite graphs on n vertices with $\kappa(G) = s(\kappa'(G) = s)$. For other undefined terminology and notation we refer to Bondy and Murty [1].

In [5], Du, Zhou and Xing determined the graphs with maximum Estrada indices among graphs with given number of cut vertices, connectivity, and edge connectivity, respectively. In this paper, we consider bipartite graphs, and characterize the unique bipartite graph with maximum Estrada indices among $\mathcal{M}_{n,p}$, $\mathcal{C}_{n,s}$ and $\mathcal{D}_{n,s}$, respectively.

2 Preliminaries

Denote by $M_k(G)$ the k-th spectral moment of a graph G, i.e., $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$. It is well-known [3] that $M_k(G)$ is equal to the number of closed walks of length k in G. Then

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

For n-vertex graphs G_1 and G_2, if $M_k(G_1) \leq M_k(G_2)$ for all positive integers k, then by Eq.(1) we have that $EE(G_1) \leq EE(G_2)$ with equality if and only if $M_k(G_1) = M_k(G_2)$ for all positive integers k.

Let k be a positive integer. For $u, v \in V(G)$, let $W_k(G; u, v)$ denote the set of (u, v)-walks of length k in G, and let $M_k(G; u, v) = |W_k(G; u, v)|$. For convenience, let $W_k(G; u) = W_k(G; u, u)$ and $M_k(G; u) = M_k(G; u, u)$.

For graphs G_1 and G_2 with $u_1, v_1 \in V(G_1)$ and $u_2, v_2 \in V(G_2)$, if $M_k(G_1; u_1, v_1) \leq M_k(G_2; u_2, v_2)$ for all positive integers k, then we write$(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$, and if $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$ and there is a positive integer k_0 such that $M_{k_0}(G_1; u_1, v_1) < M_{k_0}(G_2; u_2, v_2)$, then we write $(G_1; u_1, v_1) \prec (G_2; u_2, v_2)$. For convenience, we write $(G_1; u_1) \preceq (G_2; u_2)$ for $(G_1; u_1, u_1) \preceq (G_2; u_2, u_2)$, and $(G_1; u_1) \prec (G_2; u_2)$ for $(G_1; u_1, u_1) \prec (G_2; u_2, u_2)$.

Lemma 2.1 *[15] Let G be a graph. Then for any edge $e \notin E(G)$, one has $EE(G + e) > EE(G)$.*

Lemma 2.2 *[14] If a graph G is bipartite, and if n_0 is the nullity (=the multiplicity of its eigenvalue zero) of G, then*

$$EE(G) = n_0 + 2 \sum_{+} cosh(\lambda_i), \tag{2}$$

where cosh stands for the hyperbolic cosine $[cosh(x) = (e^x + e^{-x})/2]$, whereas $\sum_+$ denotes summation over all positive eigenvalues of the corresponding graph.

As is well known [2] that the spectrum of a complete bipartite graph K_{n_1,n_2} is $\sqrt{n_1 n_2}$, $-\sqrt{n_1 n_2}$, $0(n_1 + n_2 - 2$ times). By the definition, we have

Lemma 2.3 *[14]*
$$EE(K_{n_1,n_2}) = n_1 + n_2 - 2 + 2cosh(\sqrt{n_1 n_2}).$$

By the monotonicity of $f(x) = cosh(x)$, it is obvious that

Corollary 2.4

$$EE(K_{1,n-1}) < EE(K_{2,n-2}) < \ldots < EE(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}). \tag{3}$$

Lemma 2.5 *Let G be a non-trivial graph with $u, v \in V(G)$ such that $N_G(u) = N_G(v)$. Then for any $k \geq 0$, one has*

$$M_k(G; u) = M_k(G; v) = M_k(G; u, v) = M_k(G; v, u).$$

Proof. For any walk $W \in W_k(G; u, u)$, let $f(W)$ be the walk obtained from W by replacing its first and last vertex u by v. This is practical since $N_G(u) = N_G(v)$. Obviously, $f(W) \in W_k(G; v, v)$ and f is a bijection from $W_k(G; u, u)$ to $W_k(G; v, v)$, and so $M_k(G; u) = M_k(G; v)$. We can similarly construct a bijection from $W_k(G; u, u)$ to $W_k(G; u, v)$ or $W_k(G; v, u)$. So we have

$$M_k(G; u) = M_k(G; v) = M_k(G; u, v) = M_k(G; v, u),$$

as desired. ■

Lemma 2.6 *Let K_{n_1,n_2} be the complete bipartite graph with $X = \{x_1, x_2, \ldots, x_{n_1}\}$ and $Y = \{y_1, y_2, \ldots, y_{n_2}\}$. For any $k > 0$, one has that for any $1 \leq i, j \leq n_1$ and $1 \leq r, s \leq n_2$,*

$$M_{2k}(G; x_i, x_j) = n_1^{k-1} n_2^k \ , \qquad M_{2k}(G; y_r, y_s) = n_2^{k-1} n_1^k. \tag{4}$$

Furthermore, $M_{2k}(G) = 2(n_1 n_2)^k$.

Proof. Let $W = u_1(= x_i)u_2 \ldots u_{2k}u_{2k+1}(= x_j) \in W_{2k}(G; x_i, x_j)$ be an (x_i, x_j)-walk of length $2k$. Since G is a complete bipartite graph, it is straightforward that $u_{2r+1} \in \{x_1, x_2, \ldots, x_{n_1}\}$ and $u_{2r} \in \{y_1, y_2, \ldots, y_{n_2}\}$ for $r = 1, 2, \ldots (k-1)$. Moreover, we know that each u_{2r-1} can be arbitrarily chosen from X and each u_{2r} can be arbitrarily chosen from Y. Hence, for fixed x_i and x_j there are $n_1^{k-1} n_2^k$ walks of length $2k$ between them, that is, $M_{2k}(G; x_i, x_j) = n_1^{k-1} n_2^k$ for any $1 \leq i, j \leq n_1$. Similarly, we can obtain $M_{2k}(G; y_t, y_r) = n_2^{k-1} n_1^k$ for any $1 \leq t, r \leq n_2$. By the definition of $W_{2k}(G)$, we have

$$M_{2k}(G) = \sum_{i=1}^{n_1} M_{2k}(G; x_i) + \sum_{j=1}^{n_2} M_{2k}(G; y_j) = 2(n_1 n_2)^k.$$

The proof is complete. $\blacksquare$

Let $S_1 = \{v_1, v_2, \ldots, v_s\}$ be an independent set of G_1 and $S_2 = \{u_1, u_2, \ldots, u_s\}$ an independent set of G_2. We denote $G_1 \cup_s G_2$ as the graph obtained from G_1 and G_2 by identifying v_i with u_i for each i ($1 \leq i \leq s$). We denote the identified vertex set in $G_1 \cup_s G_2$ by S. Likewise, we can also get $G_1' \cup_s G_2'$ from G_1' and G_2', where the two independent sets that should be identified are $S_1' = \{v_1', v_2', \ldots, v_s'\}$ and $S_2' = \{u_1', u_2', \ldots, u_s'\}$, respectively.

Lemma 2.7 *Let $G = G_1 \cup_s G_2$ and $G' = G_1' \cup_s G_2'$ be the graphs of order n defined as above satisfying the following conditions:*

1. *For any $k > 0$,*
$$M_k(G_1) \leq M_k(G_1')\ , \qquad M_k(G_2) \leq M_k(G_2'); \tag{5}$$
2. *For any $1 \leq i, j \leq s$,*
$$(G_1; v_i, v_j) \preceq (G_1'; v_i', v_j')\ , \qquad (G_2; u_i, u_j) \preceq (G_2'; u_i', u_j'). \tag{6}$$

Then for any $k > 0$, $M_k(G) \leq M_k(G')$. Furthermore, $EE(G) \leq EE(G')$, with equality holds if and only if all the equalities in (5) and (6) hold.

Proof. For any $k > 0$, let $W_k(G)$ denote the set of closed walks of length k in G, we can see that

$$W_k(G) = W_k(G_1) \cup W_k(G_2) \cup W_k^3(G), \tag{7}$$

where $W_k^3(G)$ is the set of closed walks of length k in G containing both vertices in $G_1 \setminus S_1$ and vertices in $G_2 \setminus S_2$. Similarly, one has

$$W_k(G') = W_k(G_1') \cup W_k(G_2') \cup W_k^3(G'), \tag{8}$$

where $W_k^3(G')$ is the set of closed walks of length k in G' containing both vertices in $G_1' \setminus S_1'$ and vertices in $G_2' \setminus S_2'$.

By (5), we know that $|W_k(G_1)| \leq |W_k(G_1')|$ and $|W_k(G_2)| \leq |W_k(G_2')|$. We only need to show that $|W_k^3(G)| \leq |W_k^3(G')|$. In fact, there exists an injection from $W_k^3(G)$ to $W_k^3(G')$. In the following, we will construct such an injection.

For any $1 \leq i, j \leq s$, by (6) we know that for any $l > 0$,

$$M_l(G_1; v_i, v_j) \leq M_l(G_1'; v_i', v_j')\ , \quad M_l(G_2; u_i, u_j) \leq M_l(G_2'; u_i', u_j'). \tag{9}$$

So there exist an injection $f_{i,j}^l$ from $W_l(G_1; v_i, v_j)$ to $W_l(G_1'; v_i', v_j')$, and an injection $g_{i,j}^l$ from $W_l(G_2; u_i, u_j)$ to $W_l(G_2'; u_i', u_j')$ for any $1 \leq i, j \leq s$ and any $l > 0$, We will omit the subscript of $f_{i,j}^l$ and $g_{i,j}^l$ if there is no confusion about the first and last vertices of the walks we considered.

For any $W \in W_k^3(G)$, we call a maximal G_1 walk of W a 1-block, and a maximal G_2 walk of W a 2-block. From the definition, we have that the ends of a 1-block and a 2-block are both contained in S. Since $W_k^3(G)$ is the set of closed walks of length k in G_1 and contains both vertices in $G_1 \setminus S_1$ and vertices in $G_2 \setminus S_2$, there exist at least one 1-block and one 2-block, and the 1-blocks and 2-blocks appear one by one alternately with equal number. Hence we can decompose W as follows:

$$W = (B_0)B_1B_2B_3B_4 \ldots B_r, \textit{ where } r \textit{ is (odd)even},$$

where B_{2i-1} is a 1-block of length l_{2i-1}, and B_{2i} is a 2-block of length l_{2i}. We define a map φ from $W \in W_k^3(G)$ to $\varphi(W)$ as follows:

$$\varphi(W) = (g^{l_0}(B_0))f^{l_1}(B_1)g^{l_2}(B_2)f^{l_3}(B_3)g^{l_4}(B_4)\ldots.$$

Then $\varphi(W)$ is a closed walk in $W_k^3(G')$. Since both $f_{i,j}^l$ and $g_{i,j}^l$ are injection, we can easily deduce that φ is an injection. Thus, $|W_k^3(G)| \leq |W_k^3(G')|$, with equality holds if and only if for any $1 \leq i,j \leq s$ and any $l > 0$, $f_{i,j}^l$ and $g_{i,j}^l$ are bijections, that is, all the qualities in (6) hold. Hence, we have

$$\begin{aligned} M_k(G) &= |W_k(G_1)| + |W_k(G_2)| + |W_k^3(G)| \\ &\leq |W_k(G_1')| + |W_k(G_2')| + |W_k^3(G')| \\ &= M_k(G'). \end{aligned}$$

Therefore, the result follows. ∎

3 Maximum Estrada index of bipartite graphs with a given matching number

A covering of a graph G is a vertex subset $K \subseteq V(G)$ such that each edge of G has at least one end in the set K. The number of vertices in a minimum covering of a graph G is called the covering number of G and denoted by $\beta(G)$.

Lemma 3.1 (The König-Egerváry Theorem, [6, 17]). *In any bipartite graph, the number of edges in a maximum matching is equal to the number of vertices in a minimum covering.*

Let $G = G[X, Y]$ be a bipartite graph such that $G \in \mathcal{M}_{n,p}$. From Lemma 3.1, we know that $\beta(G) = p$. Let S be a minimum covering of G and $X_1 = S \cap X$, $Y_1 = S \cap Y$. Without loss of generality, suppose that $|X_1| \geq |Y_1|$ in the following analysis. Set $X_2 = X \setminus X_1$, $Y_2 = Y \setminus Y_1$. We have that $E(X_2, Y_2) = \emptyset$ since S is a covering of G.

Let $G^*[X, Y]$ be a bipartite graph with the same vertex set as G such that $E(G^*) = \{xy : x \in X_1, y \in Y\} \cup \{xy : x \in X_2, y \in Y_1\}$. Obviously, G is a subgraph of G^*. From Lemma 2.1, we know that

$$EE(G) \leq EE(G^*), \tag{10}$$

with equality holds if and only if $G \cong G^*$. Let

$$G^{**} = G^* - \{uv : u \in X_2, v \in Y_1\} + \{uw : u \in X_2, w \in X_1\},$$

Then we have the following conclusion:

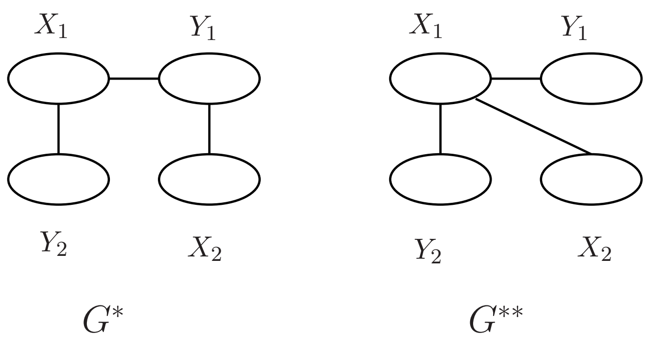

Figure 1. G^* and G^{**}

Lemma 3.2 *Let G^* and G^{**} be the graph defined above (see Figure 1). Then one has*

$$EE(G^*) \leq EE(G^{**}), \tag{11}$$

with equality holds if and only if $G^* \cong G^{**}$.

Proof. Let $G_1 = G^*[X_1, Y_2]$, $G_2 = G^*[X, Y_1]$, and $G_1' = G^{**}[X_1, Y_2]$, $G_2' = G^{**}[X_1, X_2 \cup Y_1]$. We can see that $G_1 = G_1'$, $G_2 \cong K_{|X_1|+|X_2|,|Y_1|}$ and $G_2' \cong K_{|X_1|,|Y_1|+|X_2|}$. Furthermore, $G^* = G_1 \cup_{|X_1|} G_2$, and $G^{**} = G_1' \cup_{|X_1|} G_2'$ with $S_1 = S_2 = S_1' = S_2' = X_1 = \{x_1, x_2 \ldots, x_{|X_1|}\}$.

By Lemma 2.6, we have

$$M_{2k}(G_2) = 2(|X_1| + |X_2|)^k |Y_1|^k \ , \quad M_{2k}(G_2') = 2|X_1|^k (|X_2| + |Y_1|)^k.$$

Since $|X_1| \geq |Y_1|$, we have $M_{2k}(G_2) \leq M_{2k}(G_2')$. Furthermore, as both G_2 and G_2' are bipartite graphs, one has $M_{2k-1}(G_2) = M_{2k-1}(G_2') = 0$ for any $k > 0$. Now condition 1 of Lemma 2.7 is satisfied.

For any $x_i, x_j \in X_1$, by Lemma 2.6 we know that for any $l > 0$,

$$\begin{aligned} M_{2l}(G_2; x_i, x_j) &= (|X_1| + |X_2|)^{l-1}|Y_1|^l = |Y_1|((|X_1| + |X_2|)|Y_1|)^{l-1}, \\ M_{2l}(G_2'; x_i, x_j) &= |X_1|^{l-1}(|X_2| + |Y_1|)^l = (|X_2| + |Y_1|)(|X_1|(|X_2| + |Y_1|))^{l-1}. \end{aligned}$$

As $|X_1| \geq |Y_1|$, we have $(|X_1| + |X_2|)|Y_1| \leq |X_1|(|X_2| + |Y_1|)$. Hence

$$M_{2l}(G_2; x_i, x_j) \leq M_{2l}(G_2'; x_i, x_j),$$

with equality holds if and only if $|X_2| = 0$. Together with $M_{2l-1}(G_2; x_i, x_j) = M_{2l-1}(G_2'; x_i, x_j)$ $= 0$, condition 2 of Lemma 2.7 is satisfied. So we have $EE(G^*) \leq EE(G^{**})$, with equality holds if and only if $|X_2| = 0$, i.e., $G^* \cong G^{**}$. ■

By (10) and (11), together with Corollary 2.4, it is straightforward to see that

Theorem 3.3 *Among the graphs in $\mathcal{M}_{n,p}$, $K_{p,n-p}$ is the unique graph with maximum Estrada index.*

4 Maximum Estrada index of bipartite graphs with a given connectivity(resp. edge connectivity)

For two complete bipartite graphs $K_{|X_1|,|Y_1|}$ with bipartition (X_1, Y_1) and $K_{|X_2|,|Y_2|}$ with bipartition (X_2, Y_2), we define a graph $O_s \vee_1 (K_{|X_1|,|Y_1|} \cup K_{|X_2|,|Y_2|})$, where $\cup$ is the union of two graphs, O_s ($s \geq 1$) is an empty graph of order s and $\vee_1$ is a graph operation that joins all the vertices in O_s to the vertices of X_1 and X_2 (see Figure. 2), respectively.

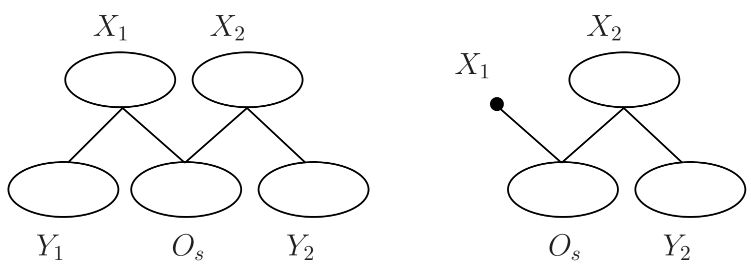

Figure 2. $O_s \vee_1 (K_{|X_1|,|Y_1|} \cup K_{|X_2|,|Y_2|})$ and $O_s \vee_1 (K_1 \cup K_{|X_2|,|Y_2|})$

Lemma 4.1 *For an n-vertex bipartite graph $O_s \vee_1 (K_1 \cup K_{p,q})$ with $p < q + s$ and $q \geq 0$, one has $EE(O_s \vee_1 (K_1 \cup K_{p,q})) < EE(O_s \vee_1 (K_1 \cup K_{q+s,p-s}))$.*

Proof. Let us denote $O_s \vee_1 (K_1 \cup K_{p,q})$ by G and $O_s \vee_1 (K_1 \cup K_{q+s,p-s})$ by G'. When there is no scope for confusion, let $O_s = \{a_1, a_2, \cdots, a_s\}$ and $V(K_1) = \{u\}$ in both G and G'.

Let $G_1 = G[\{u\}, O_s]$, $G_2 = G - \{u\}$, we can see that $G = G_1 \cup_s G_2$. Similarly, let $G'_1 = G'[\{u\}, O_s]$, $G'_2 = G' - \{u\}$, then $G' = G'_1 \cup_s G'_2$.

It is obvious that $G_1 \cong G'_1 \cong K_{1,s}$, $G_2 \cong K_{s+q,p}$ and $G'_2 \cong K_{s+p-s,q+s}$. Thus for any $k > 0$, $M_k(G_1) = M_k(G'_1)$ and for any $1 \leq i, j \leq s$, $(G_1; a_i, a_j) \preceq (G'_1; a_i, a_j)$. From Lemma 2.6, we know that $M_k(G_2) = M_k(G'_2)$ for any $k > 0$.

Moreover, by Lemma 2.6 we have that for any $l > 0$ and $1 \leq i, j \leq s$,

$$M_{2l}(G_2; a_i, a_j) = (s + q)^{l-1} p^l < (s + q)^l p^{l-1} = M_{2l}(G'_2; a_i, a_j).$$

Together with $M_{2l-1}(G_2; a_i, a_j) = 0 = M_{2l-1}(G'_2; a_i, a_j)$, we have $(G_2; a_i, a_j) \prec (G'_2; a_i, a_j)$. Hence, by Lemma 2.7 we have $EE(G) < EE(G')$, as desired. ■

Lemma 4.2 *For an n-vertex bipartite graph $O_s \vee_1 (K_1 \cup K_{p,q})$ with $p > q + s + 1$ and $q > 0$, one has $EE(O_s \vee_1 (K_1 \cup K_{p,q})) < EE(O_s \vee_1 (K_1 \cup K_{p-1,q+1}))$.*

Proof. Let X be an eigenvector of $O_s \vee_1 (K_1 \cup K_{p,q})$ corresponding to the eigenvalue λ. By the eigenvalue-equations, for any $v \in V(O_s \vee_1 (K_1 \cup K_{p,q}))$,

$$\lambda x_v = \sum_{u:uv \in E(O_s \vee_1 (K_1 \cup K_{p,q}))} x_u,$$

where x_v is the component of X corresponding to vertex v.

Thus, for any eigenvalue of $O_s \vee_1 (K_1 \cup K_{p,q})$ with $\lambda \neq 0$, one has $x_u = x_v$ if $N(u) = N(v)$. So, we can assume that

$$x_v = \begin{cases} x_1, & v \in X_1; \\ x_2, & v \in O_s; \\ x_3, & v \in X_2; \\ x_4, & v \in Y_2. \end{cases}$$

Then we know that the eigenvalue of $O_s \vee_1 (K_1 \cup K_{p,q})$ which is not equal to 0 satisfies:

$$\begin{cases} \lambda x_1 = s x_2, \\ \lambda x_2 = x_1 + p x_3, \\ \lambda x_3 = s x_2 + q x_4, \\ \lambda x_4 = p x_3. \end{cases} \tag{12}$$

As the root of (12) is also the root of

$$\lambda^4 - \lambda^2(s + pq + ps) + pqs = 0, \tag{13}$$

then we have that

$$EE(G) = n - 4 + 2cosh(\lambda_1) + 2cosh(\lambda_2),$$

where λ_1, λ_2 are the different positive roots of (13). We may assume that $r = \lambda_1 > \lambda_2$ and $k = \lambda_1\lambda_2 = \sqrt{pqs}$. Then $r > \sqrt{k} > 0$, and we can get

$$EE(O_s \vee_1 (K_1 \cup K_{p,q})) = f(r, k) = n - 4 + 2cosh(r) + 2cosh(k/r). \tag{14}$$

Then we have

$$\frac{\partial f(r,k)}{\partial r} = (e^r - e^{-r}) - \frac{k}{r^2}(e^{k/r} - e^{-k/r}) > 0, \tag{15}$$

and

$$\frac{\partial f(r,k)}{\partial k} = \frac{1}{r}(e^{k/r} - e^{-k/r}) > 0. \tag{16}$$

Let $k' = \sqrt{(p-1)(q+1)s}$. As $pqs - (p-1)(q+1)s = s(q+1-p) < 0$, we have $k < k'$.

On the other hand, let

$$g(\lambda, p, q, s) = \lambda^4 - \lambda^2(s + pq + ps) + pqs,$$

and r' be the maximum root of $g(\lambda, p-1, q+1, s)$, we will show $r' > r$. In fact, as $g(r, p, q, s) - g(r, p-1, q+1, s) = (p-q-s-1)r^2 - (p-s-1)s \geq r^2 - (p-s-1)s > 0$, we have $g(r, p-1, q+1, s) < 0$. Together with $g(\infty, p-1, q+1, s) > 0$, we can get $r' > r$. Thus, by (15) and (16) we have $f(r, k) < f(r', k')$, i.e., $EE(O_s \vee_1 (K_1 \cup K_{p,q})) < EE(O_s \vee_1 (K_1 \cup K_{p-1,q+1}))$. ■

Lemma 4.3 *For $s \leq \frac{n-3}{2}$, one has $EE(K_{s,n-s}) < EE(O_s \vee_1 (K_1 \cup K_{n-s-2,1}))$.*

Proof. By Lemma 2.3, we have $EE(K_{s,n-s}) = n-2+2cosh(\sqrt{s(n-s)})$. As in the proof of Lemma 4.2, one has

$$EE(O_s \vee_1 (K_1 \cup K_{n-s-2,1})) = n - 4 + 2cosh(\lambda_1) + 2cosh(\lambda_2),$$

where λ_1 and λ_2 are the different positive roots of

$$f(\lambda) = \lambda^4 - \lambda^2(s + (n-s-2) + (n-s-2)s) + (n-s-2)s.$$

Without loss of generality, we assume that $\lambda_1 > \lambda_2$. Then we have

$$\begin{aligned} f(\sqrt{s(n-s)}) &= -s(n^2 - 3ns - 3n + 2s^2 + 3s + 2) \\ &= -s((n-2s-3)(n-s) + 2) < 0, \end{aligned}$$

where " $<$ " holds since $s \leq \frac{n-3}{2}$, i.e., $n \geq 2s+3$. Together with $f(\infty) > 0$, we have $\lambda_1 > \sqrt{s(n-s)}$.

Now $\lambda_1 > \sqrt{s(n-s)}$, $\lambda_2 > 0$, then by the monotonicity of $cosh(\lambda)$, one has $cosh(\lambda_1) > cosh(\sqrt{s(n-s)})$ and $cosh(\lambda_2) > 1$. We then deduce

$$EE(K_{s,n-s}) < EE(O_s \vee_1 (K_1 \cup K_{n-s-2,1})),$$

as desired. ■

Lemma 4.4 *Let $G[X,Y]$ be a graph with maximum Estrada index in $\mathcal{C}_{n,s}$ and U be a minimum vertex cut. If $G-U$ has a nontrivial component G_1, then $G-U$ has exactly two components, and the other component which is distinct from G_1 cannot be nontrivial.*

Proof. Let $G_1, G_2, \ldots, G_k$ be the components of $G-U$. Suppose $k \geq 3$. Then, we can add some appropriate (at least one) edges in G between $G_1, G_2, \ldots, G_{k-1}$ so that the resulting graph G' is still bipartite. It is obvious that $G' \in \mathcal{C}_{n,s}$. By Lemma 2.1, we have $EE(G') > EE(G)$. This contradicts the fact that G has the maximum Estrada index among graphs in $\mathcal{C}_{n,s}$, and so we have $k=2$.

If both G_1 and G_2 are nontrivial with bipartition (A,B) and (C,D), respectively. Let $U = U_1 \cup U_2$ with $X = A \cup C \cup U_1$ and $Y = B \cup D \cup U_2$. Now we construct a graph $\widehat{G}$ from G by adding some edges such that $\widehat{G}[A \cup U_1, B \cup U_2]$ and $\widehat{G}[C \cup U_1, D \cup U_2]$ are both complete subgraphs. It is obvious that $EE(\widehat{G}) \geq EE(G)$. Note that $\widehat{G} \in \mathcal{C}_{n,s}$, we can assume $G = \widehat{G}$.

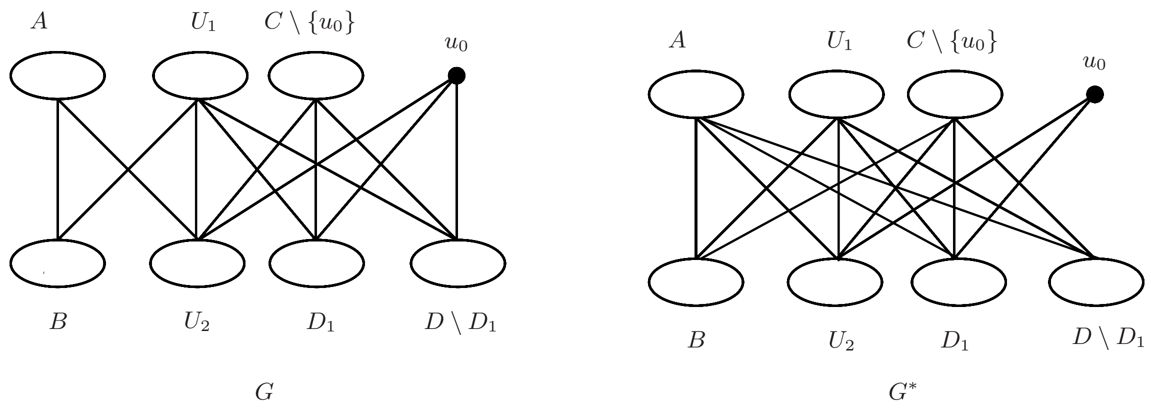

Figure 3. G and G^*

If there exists some vertex w in $G-U$ such that $d_G(w) = s$, then forming a complete bipartite graph within the vertices of $G \setminus w$ we would get a graph in $\mathcal{C}_{n,s}$ with larger

Estrada index. Thus, we may assume that each vertex in $G-U$ has a degree greater than s. We choose a vertex u_0 from C and observe that $d_G(u_0) = |U_2| + |D| > s$. Hence we have $|D| > |U_1|$.

Now choose a subset D_1 of D such that $|D_1| = |U_1|$, and let

$$G^* = G - \{u_0x : x \in D \setminus D_1\} + \{bc : b \in B, c \in C \setminus \{u_0\}\} + \{pq : p \in D, q \in A\}.$$

It is routine to check that $G^* \in \mathcal{C}_{n,s}$(see Figure 3). We claim that $EE(G) < EE(G^*)$.

For any $k > 0$ and $W = v_1v_2 \cdots v_{2k+1}(= v_1) \in W_{2k}(G)$, let $\Psi(W)$ is obtained by the following operation: For any $v_i = u_0$, we change u_0 to a if $\{v_{i-1}, v_{i+1}\} \not\subseteq D_1 \cup U_2$, where a is an arbitrary vertex of A.

It is obvious that $\Psi(W) \in W_{2k}(G^*)$ and Ψ is an injection. Hence we have for any $k > 0$, $M_{2k}(G) \leq M_{2k}(G^*)$. Together with $M_{2k-1} = M_{2k-1}(G^*) = 0$, we get $EE(G) \leq EE(G^*)$. Furthermore, as $M_2(G) = |E(G)| < |E(G^*)|$, we know that $EE(G) < EE(G^*)$, a contradiction. So, we get our conclusion. ■

Theorem 4.5 *Let $\mathcal{C}_{n,s}$ be the set of bipartite graphs on n vertices with $\kappa(G) = s$. Then*

1. *For $s \leq \frac{n-3}{2}$, the unique graph in $\mathcal{C}_{n,s}$ with the maximum Estrada index is $O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s})$.*

2. *For $\frac{n-2}{2} \leq s \leq \lfloor \frac{n}{2} \rfloor$, the unique graph in $\mathcal{C}_{n,s}$ with the maximum Estrada index is $K_{s,n-s}$.*

Proof. Let G be a graph with the maximum Estrada index in $C_{s,n}$. Let U be a vertex cut of G containing s vertices.

we distinguish the following two cases:

Case 1. All the components of $G-U$ are singletons. In this case, we have $G = K_{s,n-s}$. The result already hold for $\frac{n-2}{2} \leq s \leq \lfloor \frac{n}{2} \rfloor$. If $s \leq \frac{n-3}{2}$, by Lemma 4.3, $EE(K_{s,n-s}) < EE(O_s \vee_1 (K_1 \cup K_{n-s-2,1}))$, which contradicts the maximality of G.

Case 2. One component of $G - U$, say G_1, contains at least two vertices. By Lemma 4.4, we know that $G-U$ has exactly two components G_1 and G_2, with $G_2 \cong K_1$. Therefore, there exist p, q with $p + q + s + 1 = n, p \geq s, q > 0$, such that $G \cong O_s \vee_1 (K_1 \cup K_{p,q})$. If $\frac{n-2}{2} \leq s \leq \lfloor \frac{n}{2} \rfloor$, as $p + q + s + 1 = n, p \geq s, q > 0$, we have that $s = p = \frac{n-2}{2}, q = 1$, i.e., $G \cong O_{\frac{n-2}{2}} \vee_1 (K_1 \cup K_{\frac{n-2}{2},1})$. By Lemma 3.2, we have that $EE(G) < EE(K_{\frac{n-2}{2},\frac{n+2}{2}})$, which contradicts the maximality of G. If $s \leq \frac{n-3}{2}$, then by Lemma 4.1 and Lemma 4.2, we have $q + s \leq p \leq q + s + 1, p + q + s + 1 = n$. Hence we have $p = \lfloor \frac{n}{2} \rfloor$, i.e., $G \cong O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s})$.

We complete the proof. ■

Corollary 4.6 *Let $\mathcal{D}_{n,s}$ be the set of graphs with n vertices and edge-connectivity s. One has that for $s \leq \frac{n-3}{2}$ the unique graph in $\mathcal{D}_{n,s}$ with the maximum Estrada index is $O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s})$, and for $\frac{n-2}{2} \leq s \leq \lfloor \frac{n}{2} \rfloor$, the unique graph in $\mathcal{D}_{n,s}$ with the maximum Estrada index is $K_{s,n-s}$.*

Proof. As is well known [1] that $\kappa(G) \leq \kappa'(G)$, hence for any $G \in \mathcal{D}_{n,s}$ there exists $k \leq s$ such that $G \in \mathcal{C}_{n,k}$.

For $s \leq \frac{n-3}{2}$ we have that $k \leq \frac{n-3}{2}$. By Theorem 4.5, we have $EE(G) \leq EE(O_k \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - k})$. Since $O_k \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - k}) \subset O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s})$ as $k \leq s$, then $EE(G) \leq EE(O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s}))$.

For $\frac{n-2}{2} \leq s \leq \lfloor \frac{n}{2} \rfloor$, if $k \geq \frac{n-2}{2}$ we know that $EE(G) \leq EE(K_{k,n-k})$. By corollary 2.4 , one can easily get $EE(G) \leq EE(K_{s,n-s})$. If $k \leq \frac{n-3}{2}$, we know that $EE(G) \leq EE(O_k \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - k})) < EE(O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s}))$. By Theorem 4.5, we have $EE(O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil - 1 - s})) \leq EE(K_{s,n-s})$. The result follows. ■

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