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ON THE ESTRADA INDEX OF CACTI*

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Abstract. Let G be a simple connected graph on n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the *eigenvalues* of the adjacency matrix of G. The *Estrada index* of G is defined as $EE(G) = \Sigma_{i=1}^{n} e^{\lambda_i}$. A *cactus* is a connected graph in which any two cycles have at most one common vertex. In this work, the unique graph with maximal Estrada index in the class of all cacti with n vertices and k cycles was determined. Also, the unique graph with maximal Estrada index in the class of all cacti with n vertices and k cut edges was determined.

Key words. Eigenvalue, Estrada index, Cactus, Cut edges, Spectral moments.

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

1. Introduction. Let G be a simple graph of order n and let $A(G)$ be its adjacency matrix. The eigenvalues of G are referred as the eigenvalues of $A(G)$ and denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$. The Estrada index $EE(G)$ of the graph G is defined as $EE(G) = \Sigma_{i=1}^{n} e^{\lambda_i(G)}$. The Estrada index was introduced by Estrada [8] in 2000. Since then, the Estrada index has found 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, especially proteins [9, 10, 11] and to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks [12, 13]. Recently, the Estrada index has been received a lot of attention within mathematics. Many bounds have been established for the Estrada index in [3, 15, 16, 17, 18]. The extremal values of the Estrada index in terms of some graph invariants were also determined. Among these, Ilić and Stevanović [15] obtained 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. In [4], Du and Zhou characterized the unique unicyclic graph with maximum Estrada index, and Wang et al. [20] determine the

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unique graph with maximum Estrada index among bicyclic graphs with fixed order. Zhu et al. [19] determine the unique graph with maximum Estrada index among tricyclic graphs with fixed order. Inspired by these results, we characterize the unique graph with maximum Estrada index among cacti of fixed order.

In order to sate our results, we introduce some notation and terminology. For other notation we refer to Bollobás [1]. Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. A *cactus* is a graph in which any two cycles have at most one common vertex. If all the cycles in a cactus have exactly one common vertex, then they form a bundle. Let P_n, C_n and S_n be the path, the cycle and the star on n vertices, respectively. A *cut edge* is an edge of a graph whose removal increases the number of components of the graph. The neighborhood of a vertex v in G is $N_G(v) = \{u|uv \in E(G)\}$. Denote by $d_G(v) = |N_G(v)|$ the degree of the vertex v of G. If $d_G(v) = 1$, then v is a pendent vertex. An edge incident with the pendent vertex is a pendent edge. Let $\mathcal{C}(n, k)$ be the class of all cacti of order n with k cycles, and $\mathcal{C}(n)^k$ be the class of all cacti of order n with k cut edges.

The rest of the paper is organized as follows. In Section 2, we give some preliminaries. In Section 3, we determine the unique graph with maximal Estrada index in $\mathcal{C}(n, k)$. In Section 4, we determine the unique graph with maximal Estrada index in $\mathcal{C}(n)^k$.

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 Cvetković [2]. Then

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

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 equation (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. For any vertices u and v (not necessarily distinct) in G, we denote by $M_k(G; u, v)$ the number of walks in G with length k from u to v. Denote by $W_k(G; u, v)$ a walk of length k from u to v in G, and by $\mathcal{W}_k(G; u, v)$ the set of all such walks. Denote by $W_k(G; u, [v])$ a walk of length k from u to u which go through v in G, and by $\mathcal{W}_k(G; u, [v])$ the set of all such walks. Clearly, $M_k(G; u, v) = |\mathcal{W}_k(G; u, v)|$ and $M_k(G; u, [v]) = |\mathcal{W}_k(G; u, [v])|$. Note that $M_k(G; u, v) = M_k(G; v, u)$ for any positive integer k, see Cvetković [2].

Let G and H be graphs with $u_1,\ v_1 \in V(G)$ and $u_2,\ v_2 \in V(H)$. If $M_k(G; u_1, v_1) \leq M_k(H; u_2, v_2)$ for all positive integers, then we write $(G; u_1, v_1) \preceq (H; u_2, v_2)$. If, in addition, $M_k(G; u_1, v_1) < M_k(H; u_2, v_2)$ for at least one positive integer k, then we write $(G; u_1, v_1) \prec (H; u_2, v_2)$. If $u = v$, we write $W_k(G; u)$, $M_k(G; u)$ instead of

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$W_k(G;u,u)$, $M_k(G;u,u)$ respectively. Further, we write $(G;u)$ instead of $(G;u,u)$.

For a subset M of the edge set of the graph G, $G-M$ denotes the graph obtained from G by deleting the edges in M, and for a subset M^* of the edge set of the complement of G, $G+M^*$ denotes the graph obtained from G by inserting the edges in M^*. For $v \in V(G)$, let $G-v$ be the graph obtained from G by deleting v and its incident edges. For an edge e of the complement of G, $G+e$ denotes the graph obtained from G by inserting e.

Lemma 2.1 ([5]). *Let G be a graph containing vertices u, v. Suppose that $w_i \in V(G)$ and $uw_i \notin E(G)$, $vw_i \notin E(G)$ for $i=1,2,\ldots,k$. Let $E_u=\{uw_i, i=1,2,\ldots,k\}$ and $E_v=\{vw_i, i=1,2,\ldots,k\}$, let $G_u=G+E_u$ and $G_v=G+E_v$. If $(G;u)\prec(G;v)$ and $(G;u,w_i)\preceq G;v,w_i)$ for $i=1,2,\ldots,k$, then $EE(G_u)<EE(G_v)$.*

The *coalescence* of two vertex-disjoint connected graphs G, H denote by $G(u)\circ H(w)$, where $u\in V(G)$ and $w\in V(H)$, is obtained by identifying the vertex u of G with the vertex w of H. A graph is nontrivial if it contains at least two vertices.

Lemma 2.2 ([6]). *Let G be a connected graph containing vertices u, v and H be a nontrivial connected graph containing a vertex w. If $(G;u)\succ(G;v)$, then $EE(G(u)\circ H(w))>EE(G(v)\circ H(w))$.*

3. Graph with maximal Estrada index in $\mathcal{C}(n,k)$. In this section, we investigate the Estrada index of cacti in $\mathcal{C}(n,k)$ with n vertices and k cycles, and characterize the graphs with maximal Estrada index of $\mathcal{C}(n,k)$. First, we state some lemmas which will be used in the subsequent proofs.

Lemma 3.1. *Let Y be a nontrivial graph and H be a cycle with $u,v\in V(H)$, $w\in V(Y)$. Let $H(u)\circ Y(w)$ be the graph obtained from H and Y by identifying u with w, (see Fig. 3.1), then $(H(u)\circ Y(w);v)\prec(H(u)\circ Y(w);u)$.*

Proof. Let u_1, u_2 be the neighbors of u in H and v_1, v_2 be the neighbors of v in H, and let H_1 (H_2, respectively) be the component of $H(u)\circ Y(w)-\{uu_1,uu_2\}$ containing v ($H(u)\circ Y(w)-\{vv_1,vv_2\}$ containing u, respectively). Since Y is a nontrivial graph, then H_1 is a proper subgraph of H_2, and thus, $(H_1;v)\prec(H_2;u)$, $(H_1;v,u_1)\prec(H_2;u,v_1)$ and $(H_1;v,u_2)\prec(H_2;u,v_2)$.

Let k be a positive integer. Note that

$$M_k(H(u)\circ Y(w);v)=M_k(H_1;v)+M_k(H(u)\circ Y(w);v,[u]),$$

$$M_k(H(u)\circ Y(w);u)=M_k(H_2;u)+M_k(H(u)\circ Y(w);u,[v]).$$

Thus, we need only to show that $M_k(H(u)\circ Y(w);v,[u])<M_k(H(u)\circ Y(w);u,[v])$.

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We construct a mapping from $\mathcal{W}_k(H(u)\circ Y(w);v,[u])$ to $\mathcal{W}_k(H(u)\circ Y(w);u,[v])$. For $W\in\mathcal{W}_k(H(u)\circ Y(w);v,[u])$, we may uniquely decompose W into two sections, say W_1, W_2, where W_1 is the shortest (v,u)-section of W and W_2 is the remaining (u,v)-section of W. Note that W_1 consists of (v,u_1)-walk in H_1 and a single edge u_1u or a (v,u_2)-walk in H_1 and a single edge u_2u. Then

$$\begin{aligned}&M_k(H(u)\circ Y(w);v,[u])\\&=\sum_{\substack{k_1+k_2=k\\k_1,\ k_2\geq 1}}(M_{k_1-1}(H_1;v,u_1)+M_{k_1-1}(H_1;v,u_2))\,M_{k_2}(H(u)\circ Y(w);u,v),\\&M_k(H(u)\circ Y(w);u,[v])\\&=\sum_{\substack{k_1+k_2=k\\k_1,\ k_2\geq 1}}(M_{k_1-1}(H_2;u,v_1)+M_{k_1-1}(H_2;u,v_2))\,M_{k_2}(H(u)\circ Y(w);v,u).\end{aligned}$$

By comparing the right-hand sides of the above two equalities, we have $M_k(H(u)\circ Y(w);v,[u])<M_k(H(u)\circ Y(w);u,[v])$. □

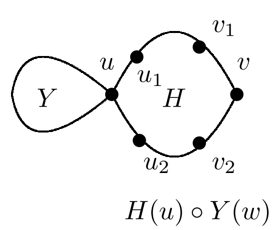

FIG. 3.1. *The graph in Lemma 3.1.*

LEMMA 3.2. *Let Y and Z be two connected graphs and X be a unicycle with disjoint vertex sets. Let u, v be two vertices on the cycle of X, $v_0\in V(Z)$, $u_0\in V(Y)$. Let G be the graph obtained from X, Y and Z by identifying v with v_0 and u with u_0, respectively, and $G^{'}$ be the graph obtained from X, Y and Z by identifying three vertices u, v_0 and u_0. $G^{''}$ is obtained from X, Y, and Z by identifying three vertices v, v_0 and u_0, (see Fig. 3.2). Then $EE(G^{'})>EE(G)$ or $EE(G^{''})>EE(G)$.*

Proof. Let $H_1=X(u)\circ Y(u_0)$ and $H_2=X(v)\circ Z(v_0)$. If $(X;u)\succ(X;v)$, then by the methods similar to the proof of Lemma 3.1, we have that $(H_1;u)\succ(H_1;v)$. Since $G\cong H_1(v)\circ Z(v_0)$ and $G^{'}\cong H_1(u)\circ Z(v_0)$, by Lemma 2.2, we have that $EE(G^{'})>EE(G)$. Otherwise, if $(X;u)\preceq(X;v)$, we have $(H_2;u)\prec(H_2;v)$, by the same reason, we have $EE(G^{''})>EE(G)$. □

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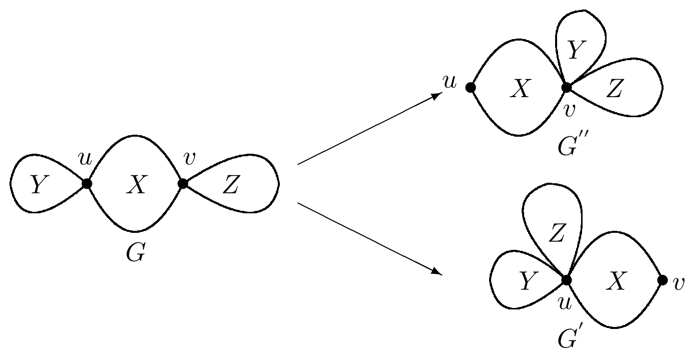

FIG. 3.2. *The graph transformation I that increase the value of Estrada index.*

LEMMA 3.3 ([6]). *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 pendent vertex to the common vertex. If $d_G(u)$, $d_G(v) \geq 2$, then $EE(G) < EE(G^{'})$.*

LEMMA 3.4. *Suppose that G is a graph of order $n \geq 6$ obtained from a connected graph J which is not isomorphic to P_1 and a cycle $C_q = u_0u_1 \cdots u_{q-1}u_0$, ($q \geq 4$) by identifying u_0 with a vertex u of the graph J, (see Fig. 3.3). Let $G^{'} = G - u_{q-1}u_{q-2} + u_0u_{q-2}$. Then $EE(G^{'}) > EE(G)$.*

Proof. Let H be the graph obtained from G by deleting the edge $u_{q-1}u_{q-2}$. First, we show that $(H; u_{q-1}) \prec (H; u_0)$. 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 $\mathcal{W}_k(H; u_{q-1})$ to $\mathcal{W}_k(H; u_0)$. For $W \in \mathcal{W}_k(H; u_{q-1})$, we may decompose W into $W = (u_{q-1}u_0)W^*(u_0u_{q-1})$, where W^* is a closed walk of length $k-2$ starting at u_0 in H. Let $f(w) = (u_0u_{q-1})(u_{q-1}u_0)W^*$, obviously, $f(W) \in \mathcal{W}_k(H; u_0)$ and f is an injection, Since $d_H(u_0) > d_H(u_{q-1}) = 1$, we have $M_2(H; u_{q-1}) < M_2(H; u_0)$. Thus, f is an injection but not a surjection for $k = 2$. It follows that $(H; u_{q-1}) \prec (H; u_0)$. Similarly, we have $(H; u_{q-2}, u_{q-1}) \prec (H; u_{q-2}, u_0)$. It can be seen easily that $G = H + u_{q-1}u_{q-2}$ and $G^{'} = H + u_0u_{q-2}$. By Lemma 2.1, we have $EE(G^{'}) > EE(G)$. This completes the proof. ◻

Let $C_0(n, k) \in \mathcal{C}(n, k)$ be a bundle of k triangles with $n - 2k - 1$ pendent vertices attached at the common vertex (see Fig. 3.4).

Now, we turn to the main result of this section. For $\mathcal{C}(n, k)$, when $k = 0$, $\mathcal{C}(n, 0)$ is the sets of all trees, when $k = 1$, $\mathcal{C}(n, 1)$ is the sets of unicyclic graphs. The following

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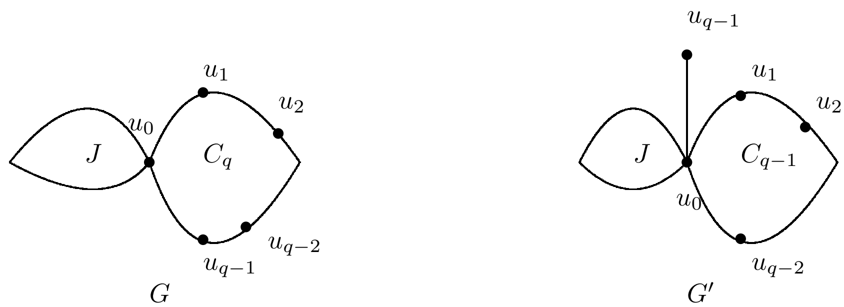

FIG. 3.3. *The graphs transformation II that increase the value of Estrada index.*

lemmas gave a sharp upper bound on the Estrada index of trees and unicyclic graphs.

LEMMA 3.5 ([7]). *Let T be a tree of order n. Then $EE(T) \leq EE(S_n)$, equality holds if and only if T is a star S_n.*

LEMMA 3.6 ([4]). *Let G be a unicyclic graph on $n \geq 4$ vertices. Then $EE(G) \leq EE(C_0(n,1))$, with equality if and only if $G \cong C_0(n,1)$.*

By Lemma 3.6, for $n = 3,\ 4,\ 5$, $C_0(n,1)$ are the graphs with maximal Estrada index in unicyclic graphs. Again for $n = 5$, $C_0(n,2)$ is the unique graph in $\mathcal{C}(5,2)$.

Next, we assume that $n \geq 6$ and $k \geq 2$.

THEOREM 3.7. *If $n \geq 6$, $k \geq 2$, then $C_0(n,k)$ is the graph in $\mathcal{C}(n,k)$ with maximal Estrada index.*

Proof. Choose $G \in \mathcal{C}(n,k)$ such that its Estrada index is maximal. We first prove that the graph G is a bundle. In order to do so we will prove the following claims.

Claim 1. Any two cycles of the graph G have one common vertex.

Proof of Claim 1. Note that any two cycles of G have no edge in common, hence, assume, on the contrary, that there are two disjoint cycles C_1 and C_2 in G. Then, we can choose cycles C_1 and C_2 such that the path P connects C_1 and C_2 is the shortest, assume that the length of P is more than 2. Let $P = u_1u_2\cdots u_p$, $(p \geq 2)$, where $u_1 \in V(C_1)$ and $u_p \in V(C_2)$ and $u_i \notin V(C_1) \cup V(C_2)$ for $i \neq 1, p$. We distinguish the following two possible cases to complete the proof of Claim 1.

Case 1. The path P (connecting C_1 and C_2) has no common edge with any other cycle(s) contained in G. By identifying the vertex u_1 with u_2 and adding a pendent edge to the common vertex u_1 (u_2), we get a graph G_1^*. By Lemma 3.3, we have $EE(G_1^*) > EE(G)$, note that $G_1^* \in \mathcal{C}(n,k)$, a contradiction to the choice of G.

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Case 2. The path P (connecting C_1 and C_2) has common edge with some other cycle, say C_3 contained in G. Note that, by the selection of C_1 and C_2, it suffices to consider that u_1 is just the common vertex of C_3 and C_1, whereas u_p is the only common vertex of C_3 and C_2. By identifying the vertex u_1 with u_p, we get a graph G_2^*. It is not hard to see that $G_2^* \in \mathcal{C}(n,k)$. By Lemma 3.2, we have $EE(G_2^*) > EE(G)$, a contradiction. This completes the proof of Claim 1. □

Claim 2. Any three cycles contained in G have exactly one common vertex.

Proof of Claim 2. Assume that in G there exist three cycles, say C_1, C_2 and C_3 such that they have no vertex in common. By Claim 1, we have in G that $V(C_1) \cap V(C_2) \neq \emptyset$, $V(C_1) \cap V(C_3) \neq \emptyset$ and $V(C_2) \cap V(C_3) \neq \emptyset$, it is easy to check that there exist two cycles in G that have common edge(s), a contradiction. □

By Claims 1 and 2, we know that all of the cycles contained in G have exactly one common vertex, say u_0. By Claims 1 and 2, we also know that the graph in $\mathcal{C}(n,k)$ having the largest Estrada index is a bundle with some pendent trees attached. Next, we are to show that if G contains a pendent tree T, then T is attached to the vertex u_0 of G.

Claim 3. Any tree T of graph G is attached to the common vertex u_0 of all cycles of the bundle.

Proof of Claim 3. Assume, to the contrary, that there exist a tree T attached to a vertex u on a cycle C of G with $u \neq u_0$. Let G_3^* be the graph obtained from G by deleting all edges of pendent tree T. For any $v \in V(G_3^*)$, by Lemma 3.1, we have $(G_3^*; u_0) \succeq (G_3^*; v)$. It is easy to see that $G \cong G_3^*(u) \circ T(u)$. Let $G_4^* \cong G_3^*(u_0) \circ T(u)$. Then by Lemma 2.2, we have $EE(G_4^*) > EE(G)$. Note that $G_4^* \in \mathcal{C}(n,k)$, contrary to the choice of G. □

Claim 4. The length of any cycle contained in G is equal to 3.

Proof of Claim 4. Suppose to the contrary that there is a cycle C with length more than 3. Let $C = u_1u_2\cdots u_pu_1$ and $p \geq 4$. Let $G_5^* = G - u_pu_{p-1} + u_1u_{p-1}$. Then $G_5^* \in \mathcal{C}(n,k)$, by Lemma 3.4, we have $EE(G_5^*) > EE(G)$, a contradiction. □

Claim 5. Let T be the tree attached to the common vertex u_0 of all the cycles contained in G, then for any $u \in V(T)\backslash u_0$, we have $d(u) = 1$.

Proof of Claim 5. Suppose to the contrary that there exist a vertex u in $V(T)\backslash u_0$ such that $d(u) \geq 2$. Let $\mathcal{N}_T^*(u)$ denote the sets of all neighbors of u in T such that $d_T(u_0,v) = d_T(u_0,u) + 1$ for each $v \in \mathcal{N}_T^*(u)$. For convenience, let v_0 be in $\mathcal{N}_T^*(u)$. Then there exist a path $P = u_0u_1\cdots uv_0$ of length more than 1 connects u_0 and v_0, where u_1 be the neighbor of u_0 in P. It is obvious that $d_G(u_1) \geq 2$ and $d_G(u_0) \geq 2$. By identifying the vertex u_0 and u_1 and appending a pendent edge to the common

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vertex u_0 (u_1), we get a graph G_6^*. By Lemma 3.3, we have $EE(G_6^*) > EE(G)$. Note that $G_6^* \in \mathcal{C}(n,k)$, contrary to the choice of G. That is to say, all edges outside of cycles are all pendent edges. □

By Claims 1 to 5, we have $G \cong C_0(n,k)$. □

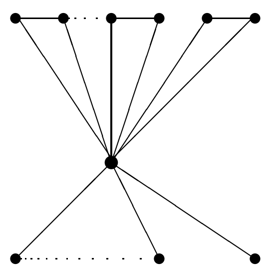

FIG. 3.4. *The graph $C_0(n,k)$ with n vertices and k cycles of length 3.*

4. Graph with maximal Estrada index in $\mathcal{C}(n)^k$. In this section, we will characterize the cacti with maximal Estrada index in terms of cut edges. We denote the set of connected cacti possessing n vertices and k cut edges by $\mathcal{C}(n)^k$.

Clearly, we have $0 \le k \le n-1$ and $k \ne n-2$. If $k = n-1$, then G is just a tree. If $0 \le k \le n-3$, then a graph in $\mathcal{C}(n)^k$ has cycles and at most $\lfloor \frac{n-k-1}{2} \rfloor$ cycles. Before proving our main result, we begin with some lemmas and preliminary results.

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

LEMMA 4.1 ([14]). *Let G be a connected graph and e be an edge of its complement. Then $EE(G) < EE(G+e)$.*

If a cactus has r (≥ 1) cycles, then we will denote these r cycles as $C_{s_1+1}, \ldots, C_{s_r+1}$ throughout the remainder of this section. We use $Cat(C_{s_1+1}, \ldots, C_{s_r+1})$ to denote a cactus obtained by taking one vertex of each C_{s_j+1}, ($1 \le j \le r$), and fusing these vertices together into a new common vertex. If we continue to attach to this new common vertex k pendent vertices, we obtain a graph, which is denoted by $Cat((C_{s_1+1}, \ldots, C_{s_r+1}), kP_2)$, (see Fig. 4.1.) for an example.

LEMMA 4.2 ([21]). *Let G be a connected graph and C_l be a cycle of G with $l \ge 5$. If there exist one vertex (denoted by u_l) at C_l of degree two and u_{l-2} is not adjacent to u_1, then there exists another graph $G' = G - u_1u_l + u_1u_{l-2}$ with a cycle C_{l-2} such*

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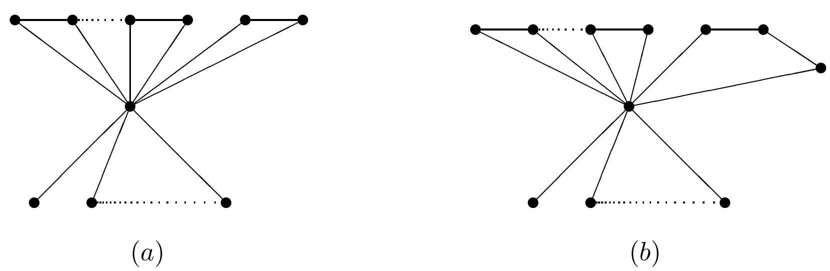

FIG. 4.1. (a) $Cat((C_3,\ldots,C_3),kP_2)$ (b) $Cat((C_3,\ldots,C_3,C_4),kP_2)$.

that $EE(G^{'}) > EE(G)$.

LEMMA 4.3. *Let* G_{max} *be the graph with the maximal Estrada index in* $\mathcal{C}(n)^k$. *Then the following hold:*
(i) *Each cut edge of* G_{max} *is pendent;*
(ii) *All cycles share exactly one common vertex* u_0*;*
(iii) *All the pendent edges of* G_{max} *are incident to the common vertex* u_0 *of* G_{max}.

Proof. (i). Suppose to the contrary that there exists a cut edge $e = uv$ which is not a pendent edge. Namely, $d_{G_{max}}(u),\ d_{G_{max}}(v) \geq 2$. By identifying the vertex u with v and appending a pendent edge to the common vertex $u(v)$, we get a graph $G^{'}$. By Lemma 3.3, we have $EE(G^{'}) > EE(G_{max})$. Note that $G^{'} \in \mathcal{C}(n)^k$, contrary to the choice of G_{max}. This establishes (i).

An argument similar to the proof of Theorem 3.7 gives (ii).

(iii). Assume to the contrary that there exist some pendent edges attached to a vertex u on a cycle C of G with $u \neq u_0$. Let G_0^* be the graph obtained from G_{max} by deleting all the pendent edges attached to u. By Lemma 3.1, we have that $(G_0^*; u_0) \succ (G_0^*; u)$. Removing all the attached pendent edges from u to u_0, we get a new graph $G^* \in \mathcal{C}(n)^k$, by Lemma 2.2, we have that $EE(G^*) > EE(G_{max})$, contrary to the choice of G_{max}. This establishes (iii). $\square$

LEMMA 4.4. *Let* G_{max} *have maximal Estrada index in* $\mathcal{C}(n)^k$, *where* $0 \leq k \leq n-3$ *and* $k = n-1$. *Then* G_{max} *contains no cycles of length greater than or equal to 5.*

Proof. We may assume without loss of generality that G_{max} has the properties mentioned in Lemma 4.3. Suppose to the contrary that there exist a cycle $C_j = u_0u_1\cdots u_{j-1}u_0$ in G_{max} with length $j \geq 5$. To obtain a contradiction, it suffices to find a graph $G \in \mathcal{C}(n)^k$ such that $EE(G) > EE(G_{max})$. Let $G^{'} = G_{max} - u_2u_3 + u_0u_3$. By Lemma 4.2, we have $EE(G^{'}) > EE(G_{max})$. Let $G_1 = G^{'} + u_0u_2$. By Lemma 4.1,

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we have $EE(G_1) > EE(G^{'})$, hence $EE(G_1) > EE(G_{max})$. Note that $G_1 \in \mathcal{C}(n)^k$ and the length of cycle C_j decreased by 2, contrary to the choice of G_{max}. □

LEMMA 4.5. *Let G_{max} have maximal Estrada index in $\mathcal{C}(n)^k$, where $0 \leq k \leq n-3$ and $k = n-1$. Then there is at most one cycle with length 4 in G_{max}.*

Proof. Suppose to the contrary that G_{max} contains two cycles of length 4. Let $C_1 = u_0u_1u_2u_3u_0$ and $C_2 = u_0u_4u_5u_6u_0$, where C_1 and C_2 share the common vertex u_0. Let $G^{'} = G_{max} - u_5u_6 + u_0u_5$. By Lemma 3.4, we get $EE(G^{'}) > EE(G_{max})$. Let $G^{''} = G^{'} - u_1u_2 + u_0u_2$. Similarly, we have $EE(G^{''}) > EE(G^{'})$. Let $G^{*} = G^{''} + u_1u_6$. By Lemma 4.1, we have $EE(G^{*}) > EE(G^{''}) > EE(G_{max})$, it is not hard to see that $G^{*} \in \mathcal{C}(n)^k$, contrary to the choice of G_{max}. □

The following theorem will determine the cacti with maximum Estrada index among graphs in $\mathcal{C}(n)^k$ for all possible values of k.

THEOREM 4.6. *For graphs in $\mathcal{C}(n)^k$ ($0 \leq k \leq n-3$ and $k = n-1$), we have:*
(i) If $k = n-1$, then the cactus S_n has the maximum Estrada index ;
(ii) If $0 \leq k \leq n-3$ and $n-k$ is odd, then $Cat((C_3, C_3, \ldots, C_3), kP_2)$ has the maximum Estrada index;
(iii) If $0 \leq k \leq n-3$ and $n-k$ is even, then $Cat((C_3, C_3, \ldots, C_3, C_4), kP_2)$ has the maximum Estrada index.

Proof. (i) is evident from Lemma 3.5. Suppose now that $0 \leq k \leq n-3$, we will prove (ii) and (iii). Let G_{max} be a graph chosen from $\mathcal{C}(n)^k$ such that for any $G \in \mathcal{C}(n)^k \backslash G_{max}$, $EE(G_{max}) \geq EE(G)$. Since G_{max} is connected and $k \leq n-3$, it must contain cycles. Assume that G_{max} contains r, $(1 \leq r \leq \lfloor \frac{n-k-1}{2} \rfloor)$ cycles, say $C_{s_1+1}, \ldots, C_{s_r+1}$. By Lemma 4.3 we know that G_{max} is isomorphic to the graph $Cat((C_{s_1+1}, \ldots, C_{s_r+1}), kP_2)$. By Lemmas 4.4 and 4.5, then there exist at most one cycle with length 4. If $r \geq 2$, all the remaining cycles are cycles with length 3 in G_{max}. Thus, G_{max} has exactly $\lfloor \frac{n-k-1}{2} \rfloor$ cycles, which implies that $G_{max} \cong Cat((C_3, \ldots, C_3), kP_2)$ if $n-k$ is odd and $G_{max} \cong Cat((C_3, \ldots, C_3, C_4), kP_2)$ if $n-k$ is even. □

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