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A Proof of a Conjecture on the Estrada Index

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Abstract

Let G be a graph on n vertices, and $\lambda_1, \lambda_2, \cdots, \lambda_n$ its eigenvalues. The Estrada index of G is a graph invariant, defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. In this paper, it is shown that the path P_n and the star S_n have the minimum and the maximum Estrada indices among n-vertex trees, respectively; and the path P_n and the complete graph K_n have the minimum and the maximum Estrada indices among connected graphs of order n, respectively. This proves a conjecture of de la Pena, Gutman and Rada.

1 Introduction

Let G be a graph with n vertices. The n eigenvalues of the adjacency matrix of G are said to be the eigenvalues of G and to form the spectrum of G; we denote these by $\lambda_1, \lambda_2, \cdots, \lambda_n$. The basic properties of graph eigenvalues can be found in the book [1].

A graph-spectrum-based molecular structure descriptor, recently put forward by Estrada [2-7], is defined as

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

Nowadays, EE is usually referred to as the Estrada index.

Although invented in year 2000, the Estrada index has already found numerous applications [2-7]. It was shown that EE is particularly suitable for characterizing the degree of folding of long-chain molecules, especially proteins [2-4]. Estrada and Rodríguez-Velázquez [5,6] showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. In a recent work [7] a connection between EE and the concept of extended atomic branching was pointed out.

Until now only some elementary general mathematical properties of the Estrada index were established [5,8-11]. One of them is the following [5,9]:

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

where $M_k = M_k(G)$ is the kth spectral moment of the graph G. As well known [1], $M_k(G)$ is equal to the number of self-returning walks of length k of the graph G. Specifically,

$$EE(G) = \sum_{k \geq 0} \frac{M_{2k}(G)}{(2k)!}$$

for a bipartite graph G.

In order to contribute towards the better understanding of the properties of the Estrada index EE and, in particular, of its dependence on the structure of the graph G, J. A. de la Peña, 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. Also, they put forward two conjectures:

Conjecture A([9]). Among n-vertex trees, P_n has the minimum and S_n the maximum Estrada index, i.e.,

$$EE(P_n) < EE(T_n) < EE(S_n)$$

where S_n and P_n denote, respectively, the n-vertex star and the n-vertex path, T_n is any n-vertex tree different from S_n and P_n.

Conjecture B([9]). Among connected graphs of order n, the path P_n has the minimum Estrada index.

Very recently, H. Zhao and Y. Jia [11] gave some new bounds for EE of bipartite graphs and proved the last inequality of Conjecture A.

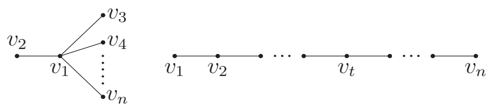
In this paper, we will give the proofs of these conjectures.

2 The Proof of Conjecture A

Let $G = (V, E)$ be a simple graph with vertex set V and edge set E. A walk in G is a finite non-null sequence $w = v_0e_1v_1e_2v_2 \cdots v_{k-1}e_kv_k$, whose terms are alternately vertices and edges, such that, for $1 \leq i \leq k$, 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 $v_1, \cdots, v_{k-1}$ its internal vertices. The integer k is the length of w. If $v_0 = v_k$, i.e., its initial and final vertices are the same, then w is called a self-returning (or closed) walk of length k of v_0. Obviously, there is no any self-returning walk with odd length in a bipartite graph.

If $w = v_0e_1v_1e_2v_2 \cdots v_{k-1}e_kv_k$ is a walk, then $w' = v_ke_kv_{k-1} \cdots v_2e_2v_1e_1v_0$ obtained by reversing w is the reverse of w, denoted by w^{-1}. A section of a walk $w = v_0e_1v_1e_2v_2 \cdots v_{k-1}e_kv_k$ is a walk that is a subsequence $v_ie_{i+1}v_{i+1} \cdots e_jv_j$ of consecutive terms of w; we refer to this subsequence as the (v_i, v_j)-section of w.

In a simple graph, a walk $v_0e_1v_1e_2v_2 \cdots v_{k-1}e_kv_k$ is determined by the sequence $v_0v_1v_2 \cdots v_{k-1}v_k$ of its vertices; hence a walk in a simple graph can be specified simply by its vertex sequence.



(a) S_n (b) P_n

Figure 1. The star S_n and the path P_n.

Lemma 1. Let S_n be the n-vertex star with vertices $v_1, v_2, \cdots, v_n$ and center v_1, depicted in Figure 1(a). Then there is an injection ξ_1 from $W_{2k}(v_2)$ to $W_{2k}(v_1)$, and ξ_1 is not surjective for $n \geq 3$ and $k \geq 1$, where $W_{2k}(v_1)$ and $W_{2k}(v_2)$ are the sets of self-returning walks of length $2k$ of v_1 and v_2 in S_n, respectively.

Proof. Let $\xi_1 : W_{2k}(v_2) \to W_{2k}(v_1)$, $\forall w \in W_{2k}(v_2)$, if $w = v_2v_1v_{i_1} \cdots v_{i_{2k-3}}v_1v_2$, then $\xi_1(w) = v_1v_2v_1v_{i_1} \cdots v_{i_{2k-3}}v_1$.

For example, in the star S_5, $\xi_1(v_2v_1v_3v_1v_2v_1v_4v_1v_2) = v_1v_2v_1v_3v_1v_2v_1v_4v_1$.

Obviously, ξ_1 is injective. However, there is no $w \in W_{2k}(v_2)$ such that

$$\xi_1(w) = v_1v_3v_1v_3v_1 \cdots v_3v_1 \in W_{2k}(v_1),$$

and ξ_1 is not surjective for $n \geq 3$ and $k \geq 1$.

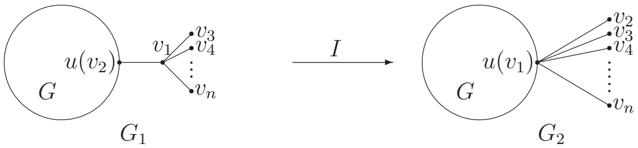


Figure 2. Transformation I.

Lemma 2. Let u be a non-isolated vertex of a simple graph G. If G_1 and G_2 are the graphs obtained from G by identifying a leaf v_2 and the center v_1 of the n-vertex star S_n to u, respectively, depicted in Figure 2, then $M_{2k}(G_1) < M_{2k}(G_2)$ for $n \geq 3$ and $k \geq 2$.

Proof. Let $W_{2k}(G)$ denote the set of self-returning walks of length $2k$ of G. Then $W_{2k}(G_i) = W_{2k}(G) \cup W_{2k}(S_n) \cup A_i$ is a partition, where A_i is the set of self-returning walks of length $2k$ of G_i, each of them contains both at least one edge in $E(G)$ and at least one edge in $E(S_n)$, $i = 1, 2$. So, $M_{2k}(G_i) = |W_{2k}(G)| + |W_{2k}(S_n)| + |A_i| = M_{2k}(G) + M_{2k}(S_n) + |A_i|$. Obviously, it is enough to show $|A_1| < |A_2|$.

Let $\eta_1 : A_1 \to A_2$, $\forall w \in A_1$, $\eta_1(w) = (w - w \cap S_n) \cup \xi_1(w \cap S_n)$, i.e., $\eta_1(w)$ is the self-returning walk of length $2k$ in A_2 obtained from w by replacing its every maximal (v_2, v_2)-section in S_n (which is a self-returning walk of v_2 in S_n) with its image under the map ξ_1.

For example,

$$\begin{aligned} & \eta_1(u_0u_1\cdots u_r\underline{v_2v_1v_3v_1v_2}u'_1\cdots u'_s\underline{v_2v_1v_4v_1v_2v_1v_5v_1v_2}u''_1\cdots u''_tu_0) \\ = \; & u_0u_1\cdots u_r\underline{v_1v_2v_1v_3v_1}u'_1\cdots u'_s\underline{v_1v_2v_1v_4v_1v_2v_1v_5v_1}u''_1\cdots u''_tu_0 \end{aligned}$$

$$\begin{aligned} & \eta_1(\underline{\underline{v_3v_1v_2}}u_1\cdots u_r\underline{v_2v_1v_4v_1v_2}u'_1\cdots u'_s\underline{\underline{v_2v_1v_4v_1v_3}}) \\ = \; & \underline{\underline{v_3v_1}}u_1\cdots u_r\underline{v_1v_2v_1v_4v_1}u'_1\cdots u'_s\underline{\underline{v_1v_2v_1v_4v_1v_3}} \end{aligned}$$

where $u_0, u_1, \cdots, u_r, u'_1, \cdots, u'_s, u''_1, \cdots, u''_t$ are vertices in G.

By Lemma 1, ξ_1 is injective. It is easily shown that η_1 is also injective. However, there is no $w \in A_1$ such that $\eta_1(w) \in A_2$ and $\eta_1(w)$ does not pass the edge v_1v_2 in G_2. So, η_1 is not surjective. And $|A_1| < |A_2|$, $M_{2k}(G_1) < M_{2k}(G_2)$.

Lemma 3. Let $P_n = v_1v_2\cdots v_n$ be the n-vertex path, depicted in Figure 1(b). Then there is an injection ξ_2 from $W'_{2k}(v_1)$ to $W'_{2k}(v_t)$, and ξ_2 is not a surjection for

$n \geq 3$, $1 < t < n$ and $k \geq 1$, where $W'_{2k}(v_1)$ and $W'_{2k}(v_t)$ are the sets of self-returning walks of length $2k$ of v_1 and v_t in P_n, respectively.

Proof. First, let $f : \{v_1, v_2, \cdots, v_t\} \to \{v_1, v_2, \cdots, v_t\}$, $f(v_i) = v_{t-i+1}$ for $i = 1, 2, \cdots, t$. Then we can induce a bijection by f from the set of self-returning walks of length $2k$ of v_1 in the sub-path $P_t = v_1 v_2 \cdots v_t$ and the set of self-returning walks of length $2k$ of v_t in P_t.

Secondly, let $\xi_2 : W'_{2k}(v_1) \to W'_{2k}(v_t)$, $\forall w \in W'_{2k}(v_1)$

(i) If w is a walk of $P_t = v_1 v_2 \cdots v_t$, i.e., w does not pass the edge $v_t v_{t+1}$, then $\xi_2(w) = f(w)$;

(ii) If w passes the edge $v_t v_{t+1}$, we can decompose w into $w = w_1 \cup w_2 \cup w_3$, where w_1 is the first (v_1, v_t)-section of w, w_3 is the last (v_t, v_1)-section of w, and the rest w_2 is the internal maximal (v_t, v_t)-section of w, i.e., w is a self-returning walk of v_1, first passing the walk w_1 from v_1 to v_t, next passing the walk w_2 from v_t to v_t, and last passing the walk w_3 from v_t to v_1; then $\xi_2(w) = w_1^{-1} \cup w_3^{-1} \cup w_2$, that is, $\xi_2(w)$ is a self-returning walk v_t, first passing the reverse of w_1 from v_t to v_1, next passing the reverse of w_3 from v_1 to v_t, and last passing the walk w_2 from v_t to v_t.

For example, in the path $P_6 = v_1 v_2 v_3 v_4 v_5 v_6$, let $t = 3$, and

$$w = v_1 v_2 v_3 v_2 v_3 v_2 v_1$$

is a self-returning walk of v_1 not passing the edge $v_3 v_4$ in P_6,

$$w' = \underline{v_1 v_2 v_3} v_2 v_1 v_2 v_3 v_4 v_5 v_4 v_3 v_2 v_1 v_2 v_3 v_4 v_3 v_2 \underline{v_3 v_2 v_1 v_2 v_1}$$

is a self-returning walk of v_1 passing the edge $v_3 v_4$ in P_6, then

$$\xi_2(w) = v_3 v_2 v_1 v_2 v_1 v_2 v_3,$$

$$\xi_2(w') = \underline{v_3 v_2 v_1 v_2 v_1 v_2 v_3} v_2 v_1 v_2 v_3 v_4 v_5 v_4 v_3 v_2 v_1 v_2 v_3 v_4 v_3 v_2 v_3.$$

Obviously, ξ_2 is injective. And ξ_2 is not surjective since there is no $w \in W'_{2k}(v_1)$ such that $\xi_2(w)$ is a self-returning walk not passing the edge $v_t v_{t-1}$ in P_n of length $2k$ of v_t.

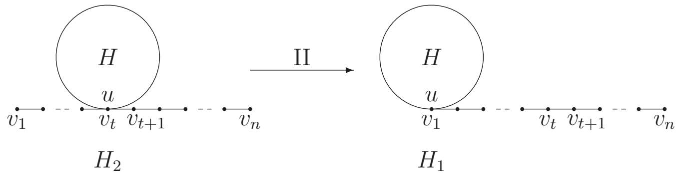


Figure 3. Transformation II.

Lemma 4. Let u be a non-isolated vertex of a simple graph H. If H_1 and H_2 are the graphs obtained from H by identifying an end vertex v_1 and the internal vertex v_t of n-vertex path P_n to u, respectively, depicted in Figure 3, then $M_{2k}(H_1) < M_{2k}(H_2)$ for $n \geq 3$ and $k \geq 2$.

Proof. Let B_i be the set of self-returning walks of length $2k$ of H_i, each of them contains both at least one edge in $E(H)$ and at least one edge in $E(P_n)$, $i = 1, 2$. Similarly to the proof of Lemma 2, it is enough to show $|B_1| < |B_2|$.

Let $\eta_2 : B_1 \to B_2$, $\forall w \in B_1$, $\eta_2(w) = (w - w \cap P_n) \cup \xi_2(w \cap P_n)$, i.e., $\eta_2(w)$ is the self-returning walk of length $2k$ in B_2 obtained from w by replacing its every section in P_n (which is a self-returning walk of v_1 in P_n) with its image under the map ξ_2.

By Lemma 3, ξ_2 is injective. It follows that η_2 is also injective. But, η_2 is not surjective since there is no $w \in B_1$ with $\eta_2(w) \in B_2$ not passing the edges $v_t v_{t-1}$ in H_2. So, $|B_1| < |B_2|$.

Theorem 5. If T_n is a n-vertex tree different from S_n and P_n, then

$$EE(P_n) < EE(T_n) < EE(S_n)$$

i.e., among n-vertex trees, P_n has the minimum and S_n the maximum Estrada index.

Proof. Repeating Transformation I as shown in Figure 2, any n-vertex tree T can be changed into the n-vertex star S_n. By Lemma 2, we have $M_{2k}(T) < M_{2k}(S_n)$ for $k \geq 2$. And

$$EE(T) = \sum_{k \geq 0} \frac{M_{2k}(T)}{(2k)!} < \sum_{k \geq 0} \frac{M_{2k}(S_n)}{(2k)!} = EE(S_n).$$

On the other hand, repeating Transformation II as shown in Figure 3, any n-vertex tree T can be changed into the n-vertex path P_n. By Lemma 4, we have

$M_{2k}(T) > M_{2k}(P_n)$ for $k \geq 2$. And

$$EE(T) = \sum_{k\geq 0} \frac{M_{2k}(T)}{(2k)!} > \sum_{k\geq 0} \frac{M_{2k}(P_n)}{(2k)!} = EE(P_n).$$

So, $EE(P_n) < EE(T_n) < EE(S_n)$.

Theorem 5 shows that Conjecture A is true.

3 The Proof of Conjecture B

Let G be a connected graph of order n and e an edge of G. The graph $G' = G - e$ is obtained from G by deleting the edge e. Obviously, any self-returning walk of length k of G' is also a self-returning walk of length k of G. Thus,

$$M_k(G') \leq M_k(G) \quad \text{and} \quad EE(G') \leq EE(G).$$

Specially, if T is a spanning tree of G, then

$$M_k(T) \leq M_k(G) \quad \text{and} \quad EE(T) \leq EE(G).$$

It follows that $EE(P_n) \leq EE(G)$ from Theorem 5. So, we have

Theorem 6. If G is a simple connected graph of order n different from the complete graph K_n and the path P_n, then

$$EE(P_n) < EE(G) < EE(K_n)$$

i.e., among all simple connected graphs of order n, P_n has the minimum and K_n the maximum Estrada index.

Theorem 6 shows that Conjecture B is true.

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