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A Note on the Estrada Index of Trees[1]

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Abstract

The trees with the fourth, fifth, and sixth greatest Estrada index are determined among all trees on n vertices, and the first six trees with the greatest Estrada index are exactly the first six trees with the greatest eigenvalue.

Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the eigenvalues of a graph G on n vertices. Then the Estrada index $EE(G)$ of G is the sum of the terms e^{λ_i}, i.e.,

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

This graph invariant appeared for the first time in year 2000, in a paper by Ernesto Estrada [1], dealing with the folding of protein molecules. Since then a remarkable variety of other chemical and non-chemical applications of EE were communicated. The mathematical studies of the Estrada index started only a few years ago. Until now a number of lower and upper bounds were obtained, and the problem of extremal EE for trees solved [2]. The relevant results on the Estrada index are surveyed in [3].

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Recently, Zhao and Jia [4] obtained the following result and determined the first three trees with the greatest Estrada index among all trees on n vertices.

Lemma 1([4]). For any two trees T_1 and T_2 on $n \geq 6$ vertices, if $T_1 \notin \{S_n^i | i = 1,2,3,4,5,6\}$, $T_2 \notin \{S_n^i | i = 1,2,3\}$, then

$$EE(S_n^1) > EE(S_n^2) > EE(S_n^3) > EE(S_n^5) > EE(S_n^6) > EE(T_1)$$

$$EE(S_n^1) > EE(S_n^2) > EE(S_n^3) > EE(T_2)$$

where S_n^i is the tree on n vertices depicted in Figure 1, $1 \leq i \leq 6$.

Note that S_n^i is also the tree with the *ith* greatest eigenvalue among all trees on n vertices [5].

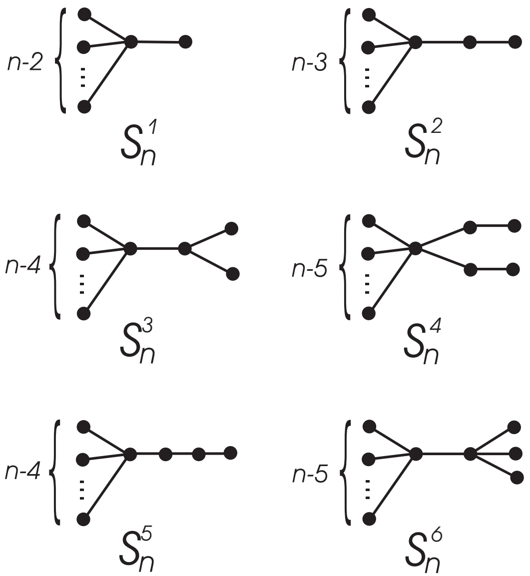

Fig. 1. Trees S_n^i , $i = 1,2,3,4,5,6$.

From Lemma 1, we know that S_n^1, S_n^2 and S_n^3 are the first three trees with the greatest Estrads index among trees on n vertices, respectively. In the following, we show that $EE(S_n^4) > EE(S_n^5)$, and S_n^i is the tree with the ith greatest Estrada index among all trees on n vertices, $i = 1, 2, 3, 4, 5, 6$.

Lemma 2. Let $P_5 = v_1v_2v_3v_4v_5$ be the path on 5 vertices. Then there is a non-surjective injection ξ from $W_{2k}(v_2)$ to $W_{2k}(v_3)$ for $k \geq 2$, where $W_{2k}(v_i)$ is the sets of self-returning walks of length $2k$ of v_i in P_5.

Proof. Let

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

be the adjacent matrix of P_5. Using induction on k, we can easily show that

$$A^{2k} = \begin{bmatrix} \frac{3^{k-1}+1}{2} & 0 & 3^{k-1} & 0 & \frac{3^{k-1}-1}{2} \\ 0 & \frac{3^k+1}{2} & 0 & \frac{3^k-1}{2} & 0 \\ 3^{k-1} & 0 & 2 \times 3^{k-1} & 0 & 3^{k-1} \\ 0 & \frac{3^k-1}{2} & 0 & \frac{3^k+1}{2} & 0 \\ \frac{3^{k-1}-1}{2} & 0 & 3^{k-1} & 0 & \frac{3^{k-1}+1}{2} \end{bmatrix}.$$

So, $|W_{2k}(v_2)| = \frac{3^k+1}{2} < |W_{2k}(v_3)| = 2 \times 3^{k-1}$ for $k \geq 2$, and there is a non-surjective injection ξ from $W_{2k}(v_2)$ to $W_{2k}(v_3)$.

Lemma 3. 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 v_2 and v_3 of the path P_5 with u, respectively, depicted in Figure 2, then $M_{2k}(G_1) < M_{2k}(G_2)$ for $k \geq 2$, where $M_k(G)$ denotes the kth spectral moment of the graph G.

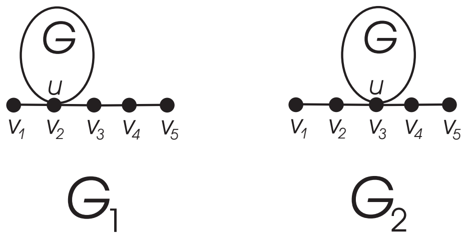

Fig. 2. The graphs G_1 and G_2.

Proof. Let $W_{2k}(G)$ denote the set of self-returning walks of length $2k$ of G. Then $W_{2k}(G_i) = W_{2k}(G) \cup W_{2k}(P_5) \cup W_i$ is a partition, where W_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 $E(P_5)$, $i = 1, 2$. So, $M_{2k}(G_i) = |W_{2k}(G)| + |W_{2k}(P_5)| + |W_i| = M_{2k}(G) + M_{2k}(P_5) + |W_i|$. Obviously, it is enough to show $|W_1| < |W_2|$.

Let $\eta : W_1 \to W_2$, $\forall x \in W_1$, $\eta(x) = (x - x \cap P_5) \cup \xi(x \cap P_5)$, i.e., $\eta(x)$ is the self-returning walk of length $2k$ in W_2 obtained from x by replacing its every self-returning walk of v_2 in P_5 with its image under the map ξ.

By Lemma 2, ξ is a non-surjective injection and so is η. And $|W_1| < |W_2|$, $M_{2k}(G_1) < M_{2k}(G_2)$.

Theorem 4. If $n \geq 6$, then $EE(S_n^4) > EE(S_n^5)$, and S_n^i is the tree with the i-th greatest Estrada index among all trees on n vertices, $i = 1, 2, 3, 4, 5, 6$.

Proof. Let $G = S_{n-4}$ be the star on $n - 4$ vertices with its center u. $G_1 = S_n^5$ and $G_2 = S_n^4$. By Lemma 3, $M_{2k}(S_n^5) < M_{2k}(S_n^4)$ for $k \geq 2$. And

$$EE(S_n^5) = \sum_{k \geq 0} \frac{M_{2k}(S_n^5)}{(2k)!} < \sum_{k \geq 0} \frac{M_{2k}(S_n^4)}{(2k)!} = EE(S_n^4) \ .$$

From Lemma 1, we know that S_n^i is the tree with the i-th greatest Estrada index among all trees on n vertices, $i = 1, 2, 3, 4, 5, 6$.

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