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Graphs with the maximal Estrada indices

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ABSTRACT

Two new transformations are proposed to compare the Estrada indices between two graphs. Let $\Psi_{n,m}$ be the set of the (n, m)-graphs, where n and m are the numbers of vertices and edges, respectively. The graphs with the maximal Estrada indices in $\Psi_{n,m}$ are deduced by the new method for three cases, namely unicyclic and bipartite unicyclic graphs ($m = n$), bicyclic graphs ($m = n + 1$), and the (n, m)-graphs without even cycles ($n + 1 \leqslant m \leqslant 3(n - 1)/2$).

1. Introduction

Let $G = (V(G), E(G))$ be a simple and connected graph with n vertices, where $V(G)$ and $E(G)$ are the sets of vertices and edges of G, respectively. The characteristic polynomial of G is $\Phi(G, \lambda) = \det[\lambda I - A(G)]$, where I is the unit matrix of order n and $A(G)$ the adjacency matrix of G [1]. The n roots of $\Phi(G, \lambda) = 0$ are denoted by $\lambda_1, \ldots, \lambda_n$. Since $A(G)$ is real and symmetric, it is obvious that each λ_i $(1 \leqslant i \leqslant n)$ is real. In order

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to study the relationship between the structure and the function of protein, the Estrada index (EI) of G, put forward by Estrada [2,3], is defined as

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

It has been found that the EI has numerical applications in biology, complex networks and chemistry. For more details, one can refer to Refs. [2–6]. Some mathematical properties of EI, including lower and upper bounds for it, may be found in Refs. [7–18]. Also the Laplacian version of EI has recently been considered [10,19–21].

For $k \geqslant 0$, we denote $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$ and refer to $M_k(G)$ as the k-th spectral moment of G. It is well known that $M_k(G)$ is equal to the number of the closed walks of length k in G [1]. From the Taylor expansion of e^{λ_i}, $EE(G)$ in (1) can be rewritten as

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \tag{2}$$

It follows from (2) that $EE(G)$ is a strictly monotonously increasing function of $M_k(G)$. Let G_1 and G_2 be two graphs. If $M_k(G_1) \geqslant M_k(G_2)$ holds for any positive integer k, then $EE(G_1) \geqslant EE(G_2)$. Moreover, if the strict inequality $M_k(G_1) > M_k(G_2)$ holds for at least one integer k, then $EE(G_1) > EE(G_2)$.

By using above-mentioned relation and constructing a mapping, the characterization of graphs with the extremal Estrada indices (EIs) has successfully been obtained. For the general trees [22], the trees with exactly two vertices having the maximal degree [23], the trees with a given matching number and the trees with a fixed diameter [24], and the trees with a given number of pendant vertices [25], etc., some interesting results were recently reported. For unicyclic graphs with n vertices, Du and Zhou [26] determined the graph with the maximal EI and showed two candidate graphs with the minimal EI. For bipartite unicyclic graphs, by constructing a relation between the EI and the largest eigenvalue of the graph, Wang [27] deduced the first four and three graphs for $n \geqslant 23$ and $22 \geqslant n \geqslant 8$, respectively. For the characterization of the graphs with the maximal EIs, Wang et al. [14] and Zhu et al. [15] recently investigated the bicyclic graphs and tricyclic graphs, respectively.

In the present study, we will deduce the graphs with the maximal EIs. The paper is organized as follows. Firstly, two new and useful transformations, namely the graph-moving transformation (see Lemma 4) and the vertex-switching transformation (see Lemma 5), are derived to compare the EIs between two connected graphs. Four theorems for studying the EIs are deduced from Lemmas 4 and 5. It is shown that some lemmas in Refs. [14] and [15] can directly be recovered from the theorems proposed in this paper. Secondly, using a simpler method than that of Du and Zhou [26], the graphs with the maximal EIs in the sets of unicyclic graphs and of bipartite unicyclic graphs will be derived for $n \geqslant 4$. Thirdly, with the aid of the two transformations, the graph with the maximal EI in the