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On extremal bipartite bicyclic graphs [☆]

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ABSTRACT

Let $\mathcal{B}_n^+$ be the set of all connected bipartite bicyclic graphs with n vertices. The Estrada index of a graph G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G, and the Kirchhoff index of a graph G is defined as $Kf(G) = \sum_{i<j} r_{ij}$, where r_{ij} is the resistance distance between vertices v_i and v_j in G. The complement of G is denoted by $\overline{G}$. In this paper, sharp upper bound on $EE(G)$ (resp. $Kf(\overline{G})$) of graph G in $\mathcal{B}_n^+$ is established. The corresponding extremal graphs are determined, respectively. Furthermore, by means of some newly created inequalities, the graph G in $\mathcal{B}_n^+$ with the second maximal $EE(G)$ (resp. $Kf(\overline{G})$) is identified as well. It is interesting to see that the first two bicyclic graphs in $\mathcal{B}_n^+$ according to these two orderings are mainly coincident.

1. Introduction

In this paper, we only consider connected, simple and undirected graphs. We follow the notations and terminology in [1,4] except otherwise stated. Throughout the text we denote by P_n, $K_{1,n-1}$ and C_n the path, star and cycle on n vertices, respectively.

Let $G = (V_G, E_G)$ be a simple and undirected graph, where V_G is the vertex set and E_G is the edge set. The *adjacency matrix* $A(G)$ of G is an $n \times n$ matrix with the (i, j)-entry equal to 1 if vertices i and j are adjacent and 0 otherwise, here $n = |V_G|$. Let $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ be the diagonal matrix of vertex degrees, where d_i is the degree of i in G for $1 \leqslant i \leqslant n$. The (*combinatorial*) *Laplacian matrix* of G is $L(G) = D(G) - A(G)$. For more information on $L(G)$ one may be referred to [23,27] and the references therein.

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In 1993, Klein and Randić [26] proposed a novel distance function, namely the *resistance distance*, on a graph. The term resistance distance is based on the following physical interpretation: one may imagine that one unit resistor on every edge of a graph G takes the resistance distance between vertices i and j of G to be the effective resistance between them, denoted by r_{ij}. The sum $Kf(G) = \sum_{i<j} r_{ij}$ was proposed in [26], later called the *Kirchhoff index* of G in [3]. It is shown [24,31] that

$$Kf(G) = \sum_{i<j} r_{ij} = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}, \tag{1.1}$$

where $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{n-1} > \mu_n = 0$ with $n \geqslant 2$ are the eigenvalues of $L(G)$. For more information on the Kirchhoff index, the readers are referred to recent papers [7,9,11,19,22] and references therein.

The *Estrada index* of a graph G is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ are the eigenvalues of $A(G)$, called the eigenvalues of G. It was first proposed as a measure of the degree of folding of a protein [16]. It was found multiple applications of Estrada index in a large variety of problems, including those in biochemistry and in complex networks, one may be referred to [17,18,20,21] for details. Various properties, especially bounds for the Estrada index have been established in [8,10,13–15].

For a simple graph G, it is hard to recognize the relationship between $EE(G)$ and $Kf(\overline{G})$ ($\overline{G}$ the complement of G) from their definitions. However, on the one hand, we know that $EE(G)$ is closely related to the numbers of closed walks in G; on the other hand, Deng and Chen [11] showed that $Kf(\overline{G})$ is closely related to the numbers of closed walk in $S(G)$ (the subdivision of G) if G is a bipartite graph. Furthermore, Deng and Chen [11] identified the first two and the last two trees according to the ordering of $Kf(\overline{T})$ by comparing the numbers of closed walks in $S(T)$, which coincide with the trees according to the ordering of $EE(T)$ for the first (resp. last) two graphs; see [8,10,25]. Recently, Deng and Chen [12] characterized the extremal connected bipartite unicyclic graphs with respect to both the Estrada index of themselves and the Kirchhoff index of their complements. They found that the first two graphs and the last one according to these two orderings are coincident. As a direct continuance of [11,12], it is interesting for us to consider extremal bipartite bicyclic graphs with respect to the above two indices at the same time.

A bicyclic graph $G = (V_G, E_G)$ is a connected simple graph which satisfies $|E_G| = |V_G| + 1$. There are two basic bicyclic graphs: ∞-graph and θ-graph. More concisely, an ∞-graph, denoted by $\infty(p, q, l)$, is obtained from two vertex-disjoint cycles C_p and C_q by connecting one vertex of C_p and one of C_q with a path P_l of length $l - 1$ (in the case of $l = 1$, identifying the above two vertices); and a θ-graph, denoted by $\theta(p, q, l)$, is a union of three internally disjoint paths P_{p+1}, P_{q+1}, P_{l+1} of length p, q, l respectively with common end vertices, where $p, q, l \geqslant 1$ and at most one of them is 1. Observe that any bicyclic graph G is obtained from an ∞-graph or a θ-graph by attaching trees to some of its vertices.

The rest of the paper is arranged as follows. In Section 2, some preliminary results are given, which include three graph operations and their properties. In Section 3, we establish the sharp upper bound on $EE(G)$ (resp. $Kf(\overline{G})$) of graph G in $\mathcal{B}_n^+$. The corresponding extremal graphs are determined, respectively. In Section 4, the graph G in $\mathcal{B}_n^+$ with the second maximal $EE(G)$ (resp. $Kf(\overline{G})$) is identified as well. In Appendix A, some new inequalities are established, which are used to prove our main results.

2. Preliminaries

In this section, we give some necessary results which will be used to prove our main results. Let G be a simple graph with n vertices and m edges and put $\overline{G}$ to be the complement of G.

In all what follows in this paper, we shall denote by $\Phi(B) = \det(xI - B)$ the *characteristic polynomial* of the square matrix B. In particular, if $B = A(G)$, we write $\Phi(A(G))$ by $\chi(G; x)$ and call $\chi(G; x)$ the *characteristic polynomial* of G; if $B = L(G)$, we write $\Phi(L(G))$ by $\sigma(G; x)$ and call $\sigma(G; x)$ the *Laplacian characteristic polynomial* of G. By [1], we have