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First and second extremal bipartite graphs with respect to PI index

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A B S T R A C T

The Padmakar–Ivan (PI) index of a graph G is defined as the sum of terms $[m_u(e) + m_v(e)]$ over all edges of G, where e is an edge, connecting the vertices u and v, where $m_u(e)$ is the number of edges of G lying closer to the vertex u than to the vertex v, and where $m_v(e)$ is defined analogously. The extremal values of the PI index are determined in the class of connected bipartite graphs with a given number of edges.

1. Introduction

Let G be a connected graph with vertex and edge sets $\mathbf{V}(G)$ and $\mathbf{E}(G)$, respectively. Suppose $u, v \in \mathbf{V}(G)$ and $e = uv \in \mathbf{E}(G)$ is the edge connecting the vertices u and v. Define the quantity $m_u(e)$ to be the number of edges lying closer to the vertex u than the vertex v. The quantity $m_v(e)$ is defined analogously. Edges equidistant from both ends of the edge uv are not counted. The Padmakar–Ivan index of G, $\mathrm{PI}(G)$, is defined as the sum of the terms $[m_u(e)+m_v(e)]$ over all edges of G; see [1–4] for details. In [5] a vertex version of this graph invariant was introduced, by which it is possible to find an exact formula for the PI index of the Cartesian product of graphs. We encourage the readers to consult [6–19] for the mathematical properties of the PI and vertex PI indices of graphs and [20,21,2] for some chemical applications and computational techniques.

Deng [7] proved that $\mathrm{PI}(G) \geq M_1(G) - 2m$, with the equality if and only if G is a complete multipartite graph. Here, m is the number of edges and $M_1(G)$ is the sum of the squares of the vertex degrees of G, usually referred to as the first Zagreb index [22–24]. He also determined the extremal graphs with respect to the PI index among all complete multipartite graphs. In [5], the authors respond to a question raised by Deng, stating that the complete graph K_n has the maximum PI index among all n-vertex graphs. The following question is still open:

Question. What is the maximum value of the PI index among n-vertex graphs?

We now consider the edge version of the above question. Suppose G is a simple graph with exactly m edges. In [8] it was shown that $\mathrm{PI}(G) \leq m(m-1)$, with equality if and only if G is a tree or an odd cycle. This shows that the maximum value of the PI index among graphs with m edges is $m(m-1)$. In view of this, it is natural to ask about the second, third, fourth, etc. extremal graphs with regard to the PI index.

The aim of this paper is to determine extremal bipartite graphs with respect to the PI index. Throughout this paper, our notation is standard and taken mainly from standard books on graph theory. Following Imrich and Klavžar [25], the Cartesian product $G \times H$ of two graphs G and H is defined on the Cartesian product $\mathbf{V}(G) \times \mathbf{V}(H)$ of the vertex sets of the

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