ARTICLE IN PRESS

Discrete Applied Mathematics ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

The weighted vertex PI index of bicyclic graphs☆

Gang Ma *, Qiuju Bian, Jianfeng Wang

School of Mathematics and Statistics, Shandong University of Technology, Zibo, Shandong, China

ARTICLE INFO

Article history:
Received 1 August 2017
Received in revised form 11 March 2018
Accepted 28 March 2018
Available online xxxx

Keywords:
Weighted vertex PI index
Bicyclic graphs

ABSTRACT

The weighted vertex PI index of a graph G is defined by

$$PI_w(G) = \sum_{e=uv\in E(G)} (d_G(u) + d_G(v))(n_u(e|G) + n_v(e|G))$$

where $d_G(u)$ denotes the vertex degree of u and $n_u(e|G)$ denotes the number of vertices in G whose distance to the vertex u is smaller than the distance to the vertex v. In this paper, we give the upper and lower bounds on the weighted vertex PI index of connected bicyclic graphs and completely characterize the corresponding extremal graphs.

1. Introduction and background

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of a shortest path between u and v in G. The length of a path or a cycle is the number of its edges. Other notations and terminologies used in the paper can be found in [1].

A topological index is a real number related to a graph. It must be a structural invariant, i.e., it preserves by every graph automorphisms. Several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.

The Wiener index is the first topological index based on graph distances [33] which was proposed in 1947. The Wiener index is defined as the sum of all distances between vertices of the graph under consideration. For more information on the Wiener index, the chemical applications of the index and its history, see [5,6,8,9]. The PI index was proposed by Khadikar [14] in 2000. The PI index is one topological index related to equidistance of vertices or parallelism of edges. It is very simple to calculate and has discriminating power in some molecular graphs. The detailed applications of PI indices between chemistry and graph theory are investigated in [4,11,15,16,19,22–25,31,36].

For each edge $e = uv \in E(G)$, let $n_u(e|G)$ be the number of vertices in G whose distance to the vertex u is smaller than the distance to the vertex v, and similarly, let $n_v(e|G)$ be the number of vertices in G whose distance to the vertex v is smaller than the distance to the vertex u. The vertex PI index of a graph G, proposed in [18], is defined as

$$PI_v(G) = \sum_{e=uv\in E(G)} [n_u(e|G) + n_v(e|G)].$$

There are nice results regarding vertex PI index in the study of computational complexity and the intersection between graph theory and chemistry, see [2,12,17,18,20,21,26,27,30,32]. One of the oldest degree-based graph invariants is the first Zagreb

☆ This work is supported by a research grant NSFC (11401348) of China.

* Corresponding author.
E-mail addresses: math_magang@163.com (G. Ma), bianqiuju@163.com (Q. Bian), jfwang@aliyun.com (J. Wang).

https://doi.org/10.1016/j.dam.2018.03.087
0166-218X/

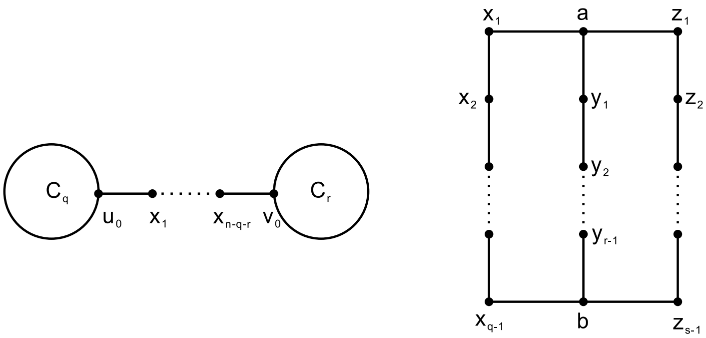

Fig. 1. Left is $\infty_n(q,r)$. Right is $B_{q,r,s}$.

indices [3,7,34], defined as follows:

$$M_1(G)=\sum_{u\in V(G)} d_G^2(u),$$

where $d_G(u)$ denotes the vertex degree of u. The vertex PI index, Zagreb indices and their variants have been used to study molecular complexity, chirality, in QSPR and QSAR analysis, see [7,16].

In order to increase diversity for bipartite graphs, Ilić and Milosavljević [13] introduce the weighted vertex PI index as follows:

$$PI_w(G)=\sum_{e=uv\in E(G)} (d_G(u)+d_G(v))(n_u(e|G)+n_v(e|G)).$$

For any edge e of a bipartite graph, $n_u(e|G)+n_v(e|G)=n$. Therefore the diversity of the vertex PI index is not satisfied for bipartite graphs. The inequality $PI_v(G)\le n\cdot m$ holds for any graph G with n vertices and m edges [18], with equality holds if and only if G is bipartite. This is why the weighted vertex PI index was introduced. If G is a bipartite graph, then

$$PI_w(G)=n\sum_{u\in V(G)} d_G^2(u).$$

This means that the weighted vertex PI index is directly connected to the first Zagreb index.

In [13], the authors show that among all connected graphs with n vertices, $PI_w(G)\ge n(4n-6)$, with equality holds if and only if $G\cong P_n$, and $PI_w(G)\le \frac{8}{27}n^4$, with equality holds if and only if $3|n$ and $G\cong K_{\frac{n}{3},\frac{n}{3},\frac{n}{3}}$. In the same paper, the exact expressions for the weighted vertex PI index of the Cartesian product of graphs are also given. In [35], the authors give the lower and upper bounds on the weighted vertex PI index of connected unicyclic graphs and characterize the corresponding extremal graphs. In [28], the exact formula for the weighted vertex PI index of corona product of two connected graphs is obtained. In [29], the exact formulas for the weighted vertex PI index of generalized hierarchical product and join of two graphs are obtained.

Denote by $\mathcal{B}_n$ the set of all connected bicyclic graphs with order n. Let $\infty_n(q,r)$ be the bicyclic graph obtained by the coalescence of two end vertices of a path $P_{n-q-r+2}$ with one vertex of two cycles C_q and C_r respectively, see left of Fig. 1. Let $P_1=P_{q+1}=x_0x_1\cdots x_q$, $P_2=P_{r+1}=y_0y_1\cdots y_r$, $P_3=P_{s+1}=z_0z_1\cdots z_s$ be three paths. Let $B_{q,r,s}$ be the bicyclic graph obtained from $P_1\cup P_2\cup P_3$ by identifying x_0,y_0,z_0 as a new vertex a, and by identifying x_q,y_r,z_s as a new vertex b, see right of Fig. 1. Clearly, any bicyclic graph must contain either graph $\infty_{n'}(q,r)$ or graph $B_{q,r,s}$ as an induced subgraph, called them *braces*. Then $\mathcal{B}_n$ can be partitioned into two subsets $\mathcal{B}_n^1$ and $\mathcal{B}_n^2$, where $\mathcal{B}_n^1$ is the set of all bicyclic graphs which contain a brace of the form $\infty_{n'}(q,r)$, and $\mathcal{B}_n^2$ is the set of all bicyclic graphs which contain a brace of the form $B_{q,r,s}$.

In Theorem 1, the upper bound on the weighted vertex PI index and the corresponding extremal graphs of bicyclic graphs are given. In Theorem 2, the lower bound on the weighted vertex PI index and the corresponding extremal graphs of bicyclic graphs are given. Let $B_{q,r,s}(a)S_{t+1}$ denote the graph obtained by identifying the vertex a of $B_{q,r,s}$ with the center of the star S_{t+1}.

Theorem 1. *For any graph $G\in\mathcal{B}_n$,*

$$PI_w(G)\le\begin{cases} n^3-n^2+24 & n\ge 9\\ n^3-3n^2+20n & 5\le n\le 8.\end{cases}$$

When $n\ge 9$, the equality holds if and only if $G\cong B_{1,2,2}(a)S_{n-3}$. When $5\le n\le 8$, the equality holds if and only if $G\cong B_{2,2,2}(a)S_{n-4}$.