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SOME GRAPHS WITH EXTREMAL PI INDEX

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Abstract

The Padmakar-Ivan (PI) index is a Wiener-Szeged-like topological index, which reflects certain structural features of organic molecules. In this paper, we study the maximum PI indices and the minimum PI indices for trees and unicyclic graphs respectively.

INTRODUCTION

The Wiener index (W) and the Szeged index (Sz) were introduced to reflect certain structural features of organic molecules [1-6]. The papers [7, 8] introduced another index, called Padmaker-Ivan (PI) index. PI index is a useful number in chemistry, as demonstrated in literature [8-16]. In [8] the authors studied the applications of the PI index to QSRP/QSAR. It turned out that the PI index has a similar discriminating power as the Wiener and Szeged indices, sometimes it gives better results. Hence, the PI index as a topological index is worth studying. In [9] the authors pointed out that the PI index is superior to ^{0}X, ^{2}X and logP indices for modeling Tadpole narcosis. In [10] the authors reported quantitative structure—toxicity relationship (QSTR) study by using the PI index. They have used 41 monosubstituted nitrobenzene for this purpose. The results have shown that the PI index alone is not an appropriate index for modeling toxicity of nitrobenzene derivatives. Combining the PI index with other distance-based topological indices resulted in statistically significant models and excellent results were obtained in pentaparametric models. For the previous results about the PI index see [17–26].

Let G be a simple connected graph. The PI index of the graph G is defined as follows:

$$PI(G) = \sum[n_{eu}(e|G) + n_{ev}(e|G)],$$

where for edge e = uv $n_{eu}(e|G)$ is the number of edges of G lying closer to u than v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than u. The summation goes over all edges of G. The edges which are equidistant from u and v are not considered for the calculation of PI index [18]. In the following we write n_{eu} instead of $n_{eu}(e|G)$.

PRELIMINARIES

For further details see [27, 28].

Definition 2.1. Let G be a graph on n vertices $v_1, v_2, \ldots, v_n$. We define G^* with parameters $p_1, p_2, \ldots, p_n$ as follows: attaching the end vertices of new paths $P_{i1}, P_{i2}, \ldots, P_{it}$ to the vertex v_i of G, let

$$p_i = t + |(E(P_{i1})| + |E(P_{i2})| + \ldots + |E(P_{it})|,$$

where i = 1, 2, …, n. If $w \in V(G^*) - V(G)$, we call w an attached vertex of G^*.

Definition 2.2. Let $v_i \in V(G)$, define

$$m_i = |\{uv \in E(G)|\ d(u, v_i) = d(v, v_i)\}|.$$

Lemma 2.3[8]. Let T be a tree with n vertices, $n \geq 2$, we have

$$PI(T) = (n - 1)(n - 2).$$

Lemma 2.4[8]. (1). Let C_{2n+1} be an odd cycle, $n \geq 1$, we have

$$PI(C_{2n+1}) = 2n(2n + 1).$$

(2). Let C_{2n} be an even cycle, $n \geq 2$, we have

$$PI(C_{2n}) = 4n(n - 1).$$

MAIN RESULTS

By Lemma 2.3 we have

Theorem 3.1. Any tree T with n vertices is an extremal graph for PI index.

Theorem 3.2. Let G be a connected unicyclic graph with n vertices, $G \neq C_n$, $G \neq C_{n-1}^*$.

(1). When n is even, we have

$$PI(C_n) < PI(G) < PI(C_{n-1}^*);$$

(2). When n is odd, we have

$$PI(C_{n-1}^*) < PI(G) < PI(C_n),$$

where C_{n-1}^* is defined in Definition 2.1 when G is C_{n-1}, that is, C_{n-1}^* is formed by attaching one new vertex of degree one to one vertex of C_{n-1}.

Proof. Claim 1: Let $y = p_1 + p_2 + \dots + p_n$, we have

$$PI(G^*) = PI(G) + y(2|E(G)| + y - 1) - (m_1p_1 + \dots + m_np_n),$$

where m_i is defined in Definition 2.2.

In fact, let $x = |E(G^*)| = |E(G)| + y$, $uv \in E(G^*) - E(G)$. By the definition of PI index we have

$$n_{eu} + n_{ev} = x - 1.$$

Hence, the total contributions of edges in $E(G^*) - E(G)$ to PI (G^*) are $y(x - 1)$.

Similarly, by the definition of PI index the total contributions of edges in E(G) to $PI(G^*)$ are

$$y|E(G)| + PI(G) - (m_1p_1 + \dots + m_np_n).$$

Hence, we have

$$PI(G^*) = PI(G) + y(2|E(G)| + y - 1) - (m_1p_1 + \dots + m_np_n).$$

Claim 1 follows.

Claim 2: Let $G = C_{2k}^*$ and $y = p_1 + p_2 + \dots + p_{2k}$, we have

$$PI(C_{2k}^*) = 4k(k-1) + y(4k + y - 1).$$

In fact, Let $uv \in E(C_{2k})$ and $v_i \in V(C_{2k})$. Let P_1 and P_2 be the shortest paths from u to v_i and v to v_i respectively, and let $z \in V(P_1) \cap V(P_2)$ be the first vertex from u to v_i along P_1. If $|E(P_1)| = |E(P_2)|$ we have

$$|E(P_1(u, z)| = |E(P_2(v, z)|.$$

Hence, we have an odd cycle

$$C = P_1(u, z) \cup P_2(v, z) \cup \{uv\},$$

which is a contradiction. Thus, we have $m_i = 0$, $i = 1, 2, \ldots, 2k$. By Claim 1 and Lemma 2.4 Claim 2 follows.

Claim 3: Let $G = C_{2k+1}^*$, $k \geq 1$, $y = p_1 + p_2 + \ldots + p_{2k+1}$, we have

$$PI(C_{2k+1}^*) = 2k(2k + 1) + y(4k + y).$$

In fact, obviously, $m_i = 1$, $i = 1, 2, \ldots, 2k + 1$. By Claim 1 and Lemma 2.4 Claim 3 follows.

Case 1. $n = 2k$.

By Lemma 2.4 we have

$$PI(C_{2k}) = 4k(k - 1).$$

By Claim 3 we have

$$PI(C_{2k-1}^*) = 4k^2 - 2k - 1.$$

When $G = C_{2x}^*$, where $x < k$,by Claim 2 we have

$$PI(C_{2x}^*) = 4x(x-1) + y(4x + y -1).$$

Since $|E(T)| = |V(T)| - 1$, where T is a tree, we have $y = 2k - 2x$.

Thus, we have

$$PI(C_{2x}^*) = 4k^2 - 2k - 2x.$$

Similarly, when $G = C_{2x+1}^*$, where $x < k - 1$,by Claim 3 we have

$$PI(C_{2x+1}^*) = 2x(2x+1) + y(4x + y).$$

Since $|E(T)| = |V(T)| - 1$, where T is a tree, we have $y = 2k - 2x - 1$.

Thus, we have

$$PI(C_{2x+1}^*) = 4k^2 - 4k + 2x + 1.$$

Hence, the first part of Theorem 3.2 follows.

Case 2. $n = 2k + 1$.

By Lemma 2.4 we have

$$PI(C_{2k+1}) = 2k(2k + 1).$$

By Claim 2 we have

$$PI(C_{2k}^*) = 4k^2.$$

When $G = C_{2x}^{*}$, where $x < k$. Similarly, we have $y = 2k - 2x + 1$. By Claim 2 we have

$$PI(C_{2x}^{*}) = 4k^2 + 2k - 2x.$$

When $G = C_{2x+1}^{*}$, where $x < k$. Similarly, we have $y = 2k - 2x$. By Claim 3 we have

$$PI(C_{2x+1}^{*}) = 4k^2 + 2x.$$

Hence, the second part of the theorem follows.

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