THEOREMS ABOUT PI INDICES

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Abstract: The Padmakar-Ivan (PI) index is a Wiener-Szeged-like topological index. In this paper we study PI index of thorn graphs, and we present a generally useful method which can reduce the computational amount of PI index strikingly.

Introduction

Wiener index (W) and Szeged index (Sz) are introduced to reflect certain structural features of organic molecules [1-6]. [7, 8] introduced another index called Padmaker-Ivan (PI) index. PI index is a very useful number in chemistry, as demonstrated in literature [8-16]. In [8] authors studied the applications of PI index to QSRP/QSAR. It turned out that the PI index has a similar discriminating function as Wiener index and Szeged index, sometimes it gave better results. Hence, PI index as a topological index is worth studying. In [9] authors pointed out that PI index is superior to ^0X, ^2X 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 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 PI index, please see [17, 18, 19, 20, 21].

Let G be a simple connected graph. The PI index of 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 and 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 $n_{eu}(e|G)$. Let $n_e = n_{eu} + n_{ev}$.

Preliminaries

For further details, see [22, 23].

Definition 2.1[24]. Let G be a graph on n vertices $v_1, v_2, \ldots, v_n$. The thorn graph of G with parameters $p_1, p_2, \ldots, p_n$, denoted by G^* or $G^*(p_1, p_2, \ldots, p_n)$, is formed by attaching p_i new vertices of degree one to the vertex v_i of G, i = 1, 2, …, n. If $w \in V(G^*) - V(G)$, we call w a thorn vertex.

Definition 2.2. Let w be a thorn vertex of G^*, $v_i \in V(G)$, $wv_i \in E(G^*)$, define

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

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]. Let P_n be a path with n vertices, $n \geq 2$. We have

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

Lemma 2.5 [8]. $PI(K_{1,n}) = n(n-1)$.

Lemma 2.6[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 $PI(C_{2n}) = 4n(n-1)$.

Lemma 2.7[8]. $PI(K_{m,n}) = mn(m+n-2)$.

Lemma 2.8[8]. For $n \geq 2$ we have

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

Lemma 2.9[22]. G is a bipartite graph if and only if G contains no odd cycle.

PI Indices of Thorn Graphs

Theorem 3.1. Let $y = p_1 + p_2 + \ldots + p_n$. We have

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

where m_i is defined in Definition 2.2.

Proof. Let $x = |E(G^*)| = |E(G)| + y$. Let w be a thorn vertex and $wv_i \in E(G^*)$. When $e = wv_i$, by the definition of PI index we have

$$n_{ew} + n_{evi} = x - 1.$$

Hence, the total contributions of edges connecting with thorn vertices of 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

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

Hence, we have

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

The theorem follows.

Theorem 3.2. Let G be a bipartite graph and $y = p_1 + p_2 + \ldots + p_n$, we have

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

Proof. Let $uv \in E(G)$ and w be a thorn vertex. Let P_1 and P_2 be the shortest paths from u to w and v to w respectively, and let $z \in V(P_1) \cap V(P_2)$ be the first vertex from u to w 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 contradicts with Lemma 2.9. Thus, we have $m_i = 0$, $i = 1, 2, \ldots, n$. By Theorem 3.1 the theorem follows.

By Theorem 3.2, Lemmas 2.3-2.7 the following theorems 3.3-3.7 are obvious, where $y = p_1 + p_2 + \ldots + p_n$.

Theorem 3.3. Let T be a tree with n vertices, $n \geq 2$, we have

$$PI(T^*) = (n - 1)(n - 2) + y(2n + y - 3).$$

Theorem 3.4. Let P_n be a path with n vertices, $n \geq 2$. We have

$$PI(P_n^*) = (n - 1)(n-2) + y(2n + y - 3).$$

Theorem 3.5. $PI(K_{1,n-1}^*) = (n - 1)(n-2) + y(2n + y - 3)$.

Theorem 3.6. Let C_{2n} be an even cycle, $n \geq 2$, we have

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

Theorem 3.7. $PI(K_{m,n}^*) = mn(m + n - 2) + y(2mn + y - 1)$.

Theorem 3.8. For $n \geq 2$, $y = p_1 + p_2 + \ldots + p_n$, we have

$$PI(K_n^*) = n(n - 1)(n - 2) + 0.5y(n^2 + n + 2y - 4).$$

Proof. By the definition of K_n we have

$$m_i = 0.5n(n - 1) - (n - 1)$$
$$= 0.5(n - 1)(n - 2).$$

By Lemma 2.8 and Theorem 3.1 the theorem follows.

Theorem 3.9. Let C_{2n+1} be an odd cycle, $n \geq 1$, $y = p_1 + p_2 + \ldots + p_{2n+1}$, we have

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

Proof. Obviously, $m_i = 1$, $i = 1, 2, \ldots, 2n + 1$. By Theorem 3.1 the theorem follows.

A General Method for the Calculations of PI Index

For a simple graph G, let Φ be a bijection: $V(G) \rightarrow V(G)$. For any pair of vertices u, v $\in V(G)$, uv $\in E(G)$ if and only if $\Phi(u)\Phi(v) \in E(G)$, we call Φ an *automorphism* of G [22].

Let G be a graph with automorphism group Γ. If Γ acts as a permutation group on V(G), we use $[\Gamma, V(G)]$ to denote the permutation group. Similarly, if Γ acts as a permutation group on E(G), we use $[\Gamma, E(G)]$ to denote the permutation group. Each permutation group $[\Gamma, X]$ partitions set X into *orbits*. If the number of orbits equals one, we say that Γ is *transitive* on X. G is a *vertex-transitive graph* if and only if Γ acts on V(G) transitively. Similarly, G is an *edge-transitive graph* if and only if Γ acts on E(G) transitively [25]. By the definitions above we have our theorem as follows:

Theorem 4.1. If edges e and f belong to the same edge orbit, we have $n_e = n_f$, where n_e and n_f are defined in section 1.

Remark: Because the edge orbits of many graphs have been determined ([25], [26]), Theorem 4.1 is a very generally useful method which can reduce the computational amount of PI index strikingly. In the following we use Theorem 4.1 to determine the PI indices of three famous graphs.

Theorem 4.2. Let G be a Petersen graph defined in [22], we have PI(G) = 180.

Proof. By the definition of edge orbit we can prove that Petersen graph has two edge orbits easily, one with 5 edges, the other with 10 edges. By the definition of PI index we have $n_e = 12$, where e is an edge in the two orbits either. By Theorem 4.1 we have PI(G) = 180. The theorem follows.

Theorem 4.3. Let G be a Folkman graph defined in [22], we have PI(G) = 1200.

Proof. Folkman proved that Folkman graph is an edge-transitive graph [22]. By the definition of PI index we have $n_e = 30$. By Theorem 4.1 we have PI(G) = 1200. The theorem follows.

Theorem 4.4. Let G be a Heawood graph defined in [22], we have PI(G) = 252.

Proof. By the definition of edge orbit we can prove that Heawood graph has two edge orbits easily, one with 14 edges, the other with 7 edges. By the definition of PI index we have $n_e = 12$, where e is an edge in the two orbits either. By Theorem 4.1 we have PI(G) = 252. The theorem follows.

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