The PI Index of the Deficient Sunflowers Attached with Lollipops

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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 PI index of the deficient sunflowers attached with lollipops.

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1 Introduction

The topological index is introduced to reflect certain structural features of organic molecules in chemical graph theory. The topological indices based on the distance of vertexes in a graph have played an important role in describing molecular graph and establish the relationship between the structure of molecular and its features in chemistry theory. At the same time it was extensively used to predict the physical and chemical properties of compounds and their biological activity. The wiener index proposed by American chemist Wiener in 1947 was the first topological index proposed [1-2]. It was used to investigate the relationship between the boiling point and its molecular structures of Alkanes. Then P.V.Khadikar proposed another topological index: the
Padmakar-Ivan (PI) index [3] which has many superior properties to wiener index [4]. The PI index of a graph $G$ is defined as follows:

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

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 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 [5].

2 Preliminary Notes

We called a vertex with degree $k$ a $k$-vertex. For further details, please see [6].

**Definition 2.1.** [7] Suppose every edge of a cycle $C_k (k \geq 3)$ is adjacent with a triangle, every triangle except the cycle $C_k$ has a 2-vertex, we called this graph a sunflower and is denoted by $SF_k$. All these triangles except $C_k$ are called the petals of this sunflower, every petal has and only has one 2-vertex.

**Definition 2.2.** When we delete $\lambda$ petals from $SF_k$, we obtain a new graph which is called deficient sunflower, denote it $DSF_{k,\lambda}$, where $\lambda$ is the number of edges in $C_k$ which are not adjacent to a triangle except $C_k$, we called $\lambda$ the deficient value of $DSF_{k,\lambda}$. Obviously, $0 \leq \lambda \leq k$. For $v_iv_{i+1} \in E(C_k)$, suppose $v_iv_{i+1}$ is adjacent with a triangle $v_iv_{i+1}u_i v_i$ except $C_k$, we say there is a petal at edge $v_iv_{i+1}$.

**Definition 2.3.** For the deficient sunflower $DSF_{k,\lambda}$, let all the vertex of $C_k$ uniformly distributed on a cycle, draw a diameter through the midpoint of edge $v_iv_{i+1}$, when $k$ is odd, this diameter must pass through a vertex $v_j$ of $C_k$, we called this vertex $v_j$ the corresponding vertex of edge $v_iv_{i+1}$. Suppose $v_j$ is a $k$-vertex, we say the corresponding vertex of edge $v_iv_{i+1}$ is a $k$-vertex. Similarly we called the edge $v_iv_{i+1}$ the corresponding edge of vertex $v_j$. When $k$ is even, this diameter must intersect with another edge $v_jv_{j+1}$ of $C_k$, we say $v_jv_{j+1}$ the corresponding edge of edge $v_iv_{i+1}$.

**Definition 2.4.** [8] Let $C_k = v_1v_2 \cdots v_kv_1, P_{n-k} = w_1w_2 \cdots w_{n-k}$. The lollipop $L(n, k)$ is obtained by connecting $v_1$ and $w_1$ with an edge $v_1w_1$, where $n > k$.

**Definition 2.5.** Attaching a lollipop graph $L(n_i, k_i)$ to each vertex $v_i$ of cycle $C_k$ in $DSF_{k,\lambda}$ and make the vertex $v_i$ coincide with the vertex $w_{n_i-k_i}$ in $L(n_i, k_i)$, attaching a lollipop graph $L(n'_i, k'_i)$ to each 2-vertex $u_i$ of a petal and make the vertex $u_i$ coincide with the vertex $w_{n'_i-k'_i}$, we get a deficient sunflower attached with lollipops and is denoted by $LDSF_{k,\lambda}$. 
We use $PI_G(H)$ to express the contributions of edges in subgraph $H$ of $G$ to the PI index of graph $G$ and use $\Delta_i$ to express the triangle $v_iv_{i+1}u_iv_i$ which is adjacent with the edge $v_iv_{i+1}$ of $C_k$. If there is a deficit at the edge of $v_iv_{i+1}$, $\Delta_i$ degenerate into an edge, then the contribution of $\Delta_i$ to the PI index of graph $G$ equals to the contribution of edge $v_iv_{i+1}$ to the PI index of graph $G$.

3 Main Results

These are the main results of the paper.

Lemma 3.1. [9] Let $T_n$ be a tree with $n$ vertices, $n \geq 2$, we have $PI(T_n) = (n-1)(n-2)$.

Lemma 3.2. [9] Let $C_n$ be a cycle with $n$ vertices, we have

$$PI(C_n) = \begin{cases} n(n-1), & n \text{ is odd;} \\ n(n-2), & n \text{ is even.} \end{cases}$$

Theorem 3.3. Let $G$ be a graph with $n$ vertices $u_1, u_2, \ldots, u_n$. We define $G'$ as follows: attaching the end vertex $w_{n_i-k_i}$ of the lollipops graph $L(n_i, k_i)$ to the vertex $u_i$, where $i=1, 2, \ldots, n$. We have

$$PI(G') = \sum_{i=1}^{n} PI_{G'}(L(n_i, k_i)) + PI(G) + N|E(G)| - (m_1n_1 + m_2n_2 + \cdots + m_nn_n)$$

where $N = n_1 + n_2 + \cdots + n_n$, $m_i = |\{xy \in E(G)|d(x, u_i) = d(y, u_i)\}|$, $t = |E(G)| + N$, $PI_{G'}(L(n_i, k_i)) = \begin{cases} (n_i-1)(t-1) + (k_i-1), & k_i \text{is odd;} \\ n_i(t-1) - k_i, & k_i \text{is even.} \end{cases}$

Proof. Obviously, when $k_i$ is odd

$$PI_{G'}(L(n_i, k_i)) = (n_i-1)(t-1) + (k_i-1).$$

When $k_i$ is even

$$PI_{G'}(L(n_i, k_i)) = k_i(t-2) + (n_i - k_i)(t-1) = n_i(t-1) - k_i.$$  

And because

$$PI_{G'}(G) = PI(G) + N|E(G)| - (m_1n_1 + m_2n_2 + \cdots + m_nn_n).$$

The theorem follows. \qed
**Theorem 3.4.** When \( k \) is even, we have

\[
PI(DSF_{k,\lambda}) = 6k^2 - 7k\lambda + 2\lambda^2 - 2\lambda.
\]

When \( k \) is odd, let the corresponding vertex of edge \( v_iv_{i+1} \) be \( v_j \), we have

\[
PI(DSF_{k,\lambda}) = 6k^2 - 7k\lambda + 2\lambda^2 + \lambda - \sum_{i=1,2,\ldots,k} d(v_j),
\]

where \( d(v_j) \) is the degree of vertex \( v_j \) in \( DSF_{k,\lambda} \).

**Proof.** Let \( x = |E(DSF_{k,\lambda})| = 3k - 2\lambda \)

Case 1. Let \( k \) be even

Subcase 1.1. \( \Delta_i \) is a degenerate triangle.

The corresponding edge \( v_{i+\frac{k}{2}}v_{i+1+\frac{k}{2}} \) of edge \( v_iv_{i+1} \) would be equidistant from \( v_i \) and \( v_{i+1} \). Other edges except \( v_iv_{i+1} \) and \( v_{i+\frac{k}{2}}v_{i+1+\frac{k}{2}} \) are not equidistant from \( v_i \) and \( v_{i+1} \). Thus, the contribution of edge \( v_iv_{i+1} \) to \( PI(DSF_{k,\lambda}) \) is \( x - 2 \).

Subcase 1.2. \( \Delta_i \) is a non-degenerate triangle.

Let \( \Delta_i \) be \( v_iv_{i+1}u_iv_i \), the corresponding edge of edge \( v_iv_{i+1} \) be \( v_jv_{j+1} \). Similar to Subcase 1.1, the contribution of \( v_iv_{i+1} \) to \( PI(DSF_{k,\lambda}) \) is \( x - 2 \). For edge \( v_iv_{i+1} \), we have

\[
d(u_i, v_i) = d(v_{i+1}, v_i),
\]

\[
d(u_i, v_{i-1}) = d(v_{i+1}, v_{i-1}),
\]

\[\vdots\]

\[
d(u_i, v_{j+1}) = d(v_{i+1}, v_{j+1}),
\]

\[
d(u_i, v_j) > d(v_{i+1}, v_j),
\]

\[
d(u_i, v_{j-1}) > d(v_{i+1}, v_{j-1}),
\]

\[\vdots\]

\[d(u_i, v_{i+2}) > d(v_{i+1}, v_{i+2}).\]

Hence, the edges whose two ends are in set \( \{v_i, u_{i-1}, v_{i-1}, \ldots, v_{j+1}, u_j\} \) are equidistant from \( v_{i+1} \) and \( u_i \). The remaining edges are not equidistant from
For edge $u_iv_i$, we have similar results. Hence, the contributions of edges in $\Delta_i$ to $PI(DF_{k,\lambda})$ are $2x$. The first half part of the theorem follows.

Case 2. Let $k$ be odd

Subcase 2.1. $\Delta_i$ is a degenerate triangle.

Let the corresponding vertex of edge $v_iv_{i+1}$ be $v_j$. Clearly, $d(v_i, v_j) = d(v_{i+1}, v_j)$. If there existed $\{u_{j-1}, u_j\} \subseteq V(DF_{k,\lambda})$, edges $v_ju_{j-1}$ and $v_ju_j$ would be equidistant from $v_i$ and $v_{i+1}$ respectively. Similarly, the edges except $v_ju_{j-1}$, $v_ju_j$ and $v_{i+1}v_i$ are not equidistant from $v_i$ and $v_{i+1}$. Hence, the contribution of edge in a degenerate triangle to $PI(DF_{k,\lambda})$ is $x - d(v_j) + 1$. There are all $\lambda$ degenerate triangles.

Subcase 2.2. $\Delta_i$ is a non-degenerate triangle.

Let $\Delta_i$ be $v_iv_{i+1}u_iv_i$, the corresponding vertex of edge $v_{i+1}v_i$ be $v_j$. When $d(v_i) = 4$, similar to Subcase 2.1 we have the contribution of edge $v_{i+1}v_i$ to $PI(DF_{k,\lambda})$ is $x - d(v_j) + 1$. For edge $u_iv_{i+1}$, similar to Subcase 1.2 we know the edges whose two ends are in set $\{v_i, u_{i-1}, v_{i-1}, \cdots v_{j+1}, u_j, v_j\}$ except $v_ju_j$ are equidistant from $v_{i+1}$ and $u_i$, the remaining edges except $u_iv_{i+1}$ are not equidistant from $v_{i+1}$ and $u_i$. For edge $u_iv_{i+1}$, we have similar results. Hence, the sum of the contributions of edges $u_iv_i$ and $u_{i+1}v_i$ to $PI(DF_{k,\lambda})$ equals $x + d(v_j) - 1$. Thus, the contributions of edges in $\Delta_i$ to $PI(DF_{k,\lambda})$ are $2x$. When $d(v_i) = 3$ and $d(v_i) = 2$, we can discuss similarly. Hence,

$$PI(DF_{k,\lambda}) = 2x(k - \lambda) + \sum_{i=1,2,\ldots,k, \text{no petal at } v_{i+1}} (x - d(v_j) + 1)$$

Substitute $3k - 2\lambda$ to $x$. The theorem follows. \hfill \Box

For the deficient sunflower attached with lollipops $LDSF_{k,\lambda}$ defined in definition 2.5, in the following let $N = (n_1 + n_2 + \cdots + n_k) + (n_1' + n_2' + \cdots + n_k')$, $x = |E(DF_{k,\lambda})| = 3k - 2\lambda$, $t = x + N$.

**Theorem 3.5.** Let $S = |\{k_i | k_i \text{ is odd} \} \cup \{k'_i | k'_i \text{ is odd} \}|$, $P = \sum_{i=1}^{k} k_i$ + $\sum_{i=1}^{k} k'_i$, $Q = \sum_{i=1}^{k} k_i + \sum_{i=1}^{k} k'_i$. $PI(DF_{k,\lambda})$ is provided by Theorem 3.2.

When $k$ is odd, let the corresponding edge of vertex $v_i$ be $v_{i+1}v_j$ and

$$T = (2k - \lambda)N - \sum_{i=1,2,\ldots,k, \text{no petal at } v_{i+1}} n_i.$$  

When $k$ is even, let the corresponding edge of edge $v_{i+1}v_i$ be $v_{j+1}v_j$ and

$$T = (2k - \lambda)N - \sum_{i=1,2,\ldots,k, \text{no petal at } v_{i+1}} n'_i.$$
We have

$$PI(L_{DSF}, k, \lambda) = Q - tS - P + (t - 1)N + PI(DSF, k, \lambda) + T.$$ 

**Proof.** Let $M = Q - S$, $M' = P(t - 2)$, $M'' = (t - 1)(N - S - P)$.

Claim 1. $\sum_{i=1}^{k} PI(L_{DSF}, k, \lambda)[L(n_i, k_i)] + \sum_{i=1}^{k} PI(L_{DSF}, k, \lambda)[L(n_i', k_i')] = M + M' + M''$

In fact, we can classify all the edges of lollipops $L(n_i, k_i)$ and $L(n_i', k_i')$ in $L_{DSF}$ into three classes according to their contributions to $L_{DSF}$.

If $k_i$ (or $k_i'$) is odd, the contribution of the corresponding edge of vertex $w_1$ in $C_{k_i}$ (or $C_{k_i'}$) to $PI(L_{DSF})$ is $k_i - 1$ (or $k_i' - 1$). All these edges are in the first class. The sum of the contributions of all these edges to $PI(L_{DSF})$ are

$$\sum_{i=1, k_i \text{ is odd}}^{k} (k_i - 1) + \sum_{i=1, k_i' \text{ is odd}}^{k} (k_i' - 1) = M.$$ 

If $k_i$ (or $k_i'$) is even, the contribution of every edge in $C_{k_i}$ (or $C_{k_i'}$) to $PI(L_{DSF})$ is $t - 2$. All these edges are in the second class. The sum of the contributions of all these edges to $PI(L_{DSF})$ are

$$(t - 2)(\sum_{i=1, k_i \text{ is even}}^{k} k_i + \sum_{i=1, k_i' \text{ is even}}^{k} k_i') = M'.$$

The other edges except the edges in class one and class two are in the third class. Each of them has $t - 1$ contribution to $PI(L_{DSF})$. The sum of the contributions of all these edges to $PI(L_{DSF})$ are

$$(t - 1)[N - S - (\sum_{i=1, k_i \text{ is even}}^{k} k_i + \sum_{i=1, k_i' \text{ is even}}^{k} k_i')] = M''.$$

Thus Claim 1 follows.

Claim 2. Let $m_i$ and $m_i'$ be defined in Theorem 3.1. When $k$ is odd, let the corresponding edge of vertex $v_i$ be $v_{j_1}v_{j_1+1}$, we have

$$m_i' = k - \lambda; m_i = k - \lambda + 1$$

if there is a petal at $v_{j_1}v_{j_1+1}$, $m_i = k - \lambda + 1$ if there is no petal at $v_{j_1}v_{j_1+1}$.

When $k$ is even, let the corresponding edge of edge $v_{i_1}v_{i_1+1}$ be $v_{j_1}v_{j_1+1}$, we have

$$m_i = k - \lambda; m_i' = 0$$

if $n_i' > 0$ or $m_i' = k - \lambda + 1$ if there is no petal at $v_{j_1}v_{j_1+1}$, $m_i' = k - \lambda + 1$ if there is no petal at $v_{j_1}v_{j_1+1}$.

In fact, we can prove Claim 2 as follows:

Case 2.1. $k$ is odd.
For the vertex $u_i \in V(DSF_{k,\lambda})$, there existed one and only one edge in each petal whose two ends are equidistant from $u_i$. Thus $m_i' = k - \lambda$.

For the vertex $v_i \in V(DSF_{k,\lambda})$, clearly, $d(v_j, v_i) = d(v_{j+1}, v_i)$. Other petals except the one at $v_jv_{j+1}$ have and only have one edge whose two ends are equidistant from $v_i$.

Case 2.2. $k$ is even.

We can get the conclusion similar to Case 2.1. Thus, Claim 2 follows.

By Theorem 3.1 the theorem follows.

\[ \square \]

References


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