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The PI index of bridge and chain graphs

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Abstract

The Padmakar-Ivan (PI) index of a graph G is the sum over all edges uv of G of the number of edges which are not equidistant from the vertices u and v. In this paper, we compute the PI index of bridge and chain graphs. Using these formulas, the PI indices of several graphs are computed.

1. Introduction

In theoretical chemistry molecular structure descriptors - also called topological indices - are used to understand physico-chemical properties of chemical compounds. By now there do exist a lot of different types of such indices which capture different aspects of the molecular graphs associated to the molecules considered. Arguably the most famous such index is the Wiener index [10, 20]. The Szeged index [9, 13] is closely related to the Wiener index and is a vertex-multiplicative type index that takes into account how the vertices of a given molecular graph are distributed. The Padmakar-Ivan index [12, 15] is an additive index that takes into account the distribution of edges and, therefore, complements the Szeged index in a certain sense. It is useful to mention that the PI index is the unique topological index related to parallelism of edges (we will make this more precise below).

In [18] many chemical applications of the PI index were presented and it was shown that the PI index correlates highly with the Wiener and Szeged index as well as with the physico-chemical properties and biological activities of a large number of diverse and complex compounds. The PI index has been studied from many different point of views, see [1]-[8], [11, 12] and [14]-[18]. Let us point out that Klavzar [19] computed the PI index for Cartesian product graphs. This result was independently obtained in [5].

In this paper we compute the PI index for several families of graphs, including the bridge graph and the chain graph built from a collection of (possibly different) graphs.

2. Preliminaries

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, we denote the distance between two arbitrary vertices x and y of G by $d(x, y)$ and it is defined as the number of edges in the minimal path connecting the vertices x and y.

Given an edge $e = uv \in E(G)$ of G, we define the distance of e to a vertex $w \in V(G)$ as the minimum of the distances of its edges to w, i.e.,

$$d(w, e) := \min\{d(w, u), d(w, v)\}.$$

Let us denote the number of edges lying closer to the vertex u than the vertex v of e by $n_{eu}(e|G)$ and the number of edges lying closer to the vertex v than the vertex u by $n_{ev}(e|G)$. Thus,

$$n_{eu}(e|G) := |\{f \in E(G) \,|\, d(u, f) < d(v, f)\}|$$

and similarly for $n_{ev}(e|G)$.

The *Padmakar-Ivan (PI) index* of a graph G is defined as

$$PI(G) := \sum_{e \in E(G)} (n_{eu}(e|G) + n_{ev}(e|G)),$$

see [12, 14, 15, 16, 17, 18]. Note that in this definitions the edges equidistant from the two ends of the edge $e = uv$ - i.e., edges f with $d(u, f) = d(v, f)$ - are not counted. We call such edges *parallel* to e. This implies that we can write

$$PI(G) = \sum_{e \in E(G)} n_e(G),$$

where $n_e(G) := n_{eu}(e|G) + n_{ev}(e|G)$ is the number of edges of G that are not equidistant from the two ends of the edge e.

3. The bridge Graph

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The *bridge graph*

$$B(G_1, G_2, \ldots, G_d) = B(G_1, G_2, \ldots, G_d; v_1, v_2, \ldots, v_d)$$

of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, \ldots, G_d$ by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \ldots, d-1$, see Figure 1.

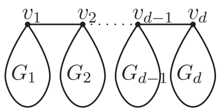

Figure 1. The bridge graph

In order to compute the PI index of the bridge graph $B(G_1, G_2, \ldots, G_d)$ we need the following notation. Let G be any graph and let $v \in V(G)$ be any vertex of G. We denote the set of all edges uu' such that $d(u, v) = d(u', v)$ by $M_v(G)$. The cardinality of $M_v(G)$ is denoted by $m_v(G)$.

Theorem 1. *The PI index of the bridge graph $G = B(G_1, G_2, \ldots, G_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is given by*

$$PI(G) = 1 + \sum_{i=1}^{d}(PI(G_i) - 1) + |E(G)|(|E(G)| - m(G)) - \sum_{i=1}^{d} |E(G_i)|(|E(G_i)| - m_{v_i}(G_i))$$

where $m(G) := \sum_{i=1}^d m_{v_i}(G_i)$.

Proof. Let $G = B(G_1, G_2, \ldots, G_d)$. From the definitions we have that

$$\begin{aligned} PI(G) &= \sum_{e\in E(G)} n_e(G) \\ &= \sum_{i=1}^{d} \sum_{e\in E(G_i)} n_e(G) + \sum_{i=1}^{d-1} n_{v_i v_{i+1}}(G) \\ &= \sum_{i=1}^{d} \sum_{e\in M_{v_i}(G_i)} n_e(G) + \sum_{i=1}^{d} \sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} n_e(G) + \sum_{i=1}^{d-1} n_{v_i v_{i+1}}(G). \end{aligned}$$

If e is the edge $v_i v_{i+1}$ in G then no other edge f is equidistant from the ends of the edge e, thus $n_e(G) = |E(G)| - 1$. This implies that

$$PI(G) = \sum_{i=1}^{d} \sum_{e\in M_{v_i}(G_i)} n_e(G) + \sum_{i=1}^{d} \sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} n_e(G) + (d-1)(|E(G)| - 1).$$

If $e \in M_{v_i}(G_i)$ then all the edges in $E(G) \setminus E(G_i)$ are equidistant from the ends of the edge e, thus $n_e(G) = n_e(G_i)$, yielding in turn

$$PI(G) = \sum_{i=1}^{d} \sum_{e\in M_{v_i}(G_i)} n_e(G_i) + \sum_{i=1}^{d} \sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} n_e(G) + (d-1)(|E(G)| - 1).$$

If $e \in E(G_i) \setminus M_{v_i}(G_i)$ then each edge in $E(G) \setminus E(G_i)$ is not equidistant from the ends of the edge e, thus $n_e(G) = n_e(G_i) + |E(G)| - |E(G_i)|$ and, consequently,

$$\begin{aligned} PI(G) = & \sum_{i=1}^{d} \sum_{e\in M_{v_i}(G_i)} n_e(G_i) + \sum_{i=1}^{d} \sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} (n_e(G_i) + |E(G)| - |E(G_i)|) \\ & +(d-1)(|E(G)| - 1). \end{aligned}$$

This is equivalent to

$$\begin{aligned} & PI(G) \\ &= \sum_{i=1}^{d} \sum_{e\in E(G_i)} n_e(G_i) + \sum_{i=1}^{d} \sum_{e\in E(G_i)\setminus M_{v_i}(G_i)} (|E(G)| - |E(G_i)|) + (d-1)(|E(G)| - 1) \\ &= \sum_{i=1}^{d} PI(G_i) + \sum_{i=1}^{d} (|E(G_i)| - m_{v_i}(G_i))(|E(G)| - |E(G_i)|) + (d-1)(|E(G)| - 1) \\ &= 1 + \sum_{i=1}^{d} (PI(G_i) - 1) + |E(G)|(|E(G)| - m(G)) - \sum_{i=1}^{d} |E(G_i)|(|E(G_i)| - m_{v_i}(G_i)), \end{aligned}$$

as claimed. □

Define

$$G_d(H,v) = B(\underbrace{H,H,\ldots,H}_{d \text{ times}},\underbrace{v,v,\ldots,v}_{d \text{ times}}).$$

Clearly, $G_1(H,v) = H$ for any vertex v of H. As a corollary of Theorem 1 we have the following result.

Corollary 2. *Let H be any graph with fixed vertex v. Then the PI index of the bridge graph $G_d(H,v)$ is given by*

$$PI(G_d(H,v)) = dPI(H) + (d-1)\Big(d(|E(H)|+1)(|E(H)|+1-m_v(H)) - 2\Big).$$

Proof. Let $G = G_d(H,v)$. Theorem 1 for the bridge graph G gives that

$$PI(G) = 1 + \sum_{i=1}^{d}(PI(H)-1) + |E(G)|(|E(G)| - m(G)) - \sum_{i=1}^{d}|E(H)|(|E(H)| - m_v(H))$$

which is equivalent to

$$PI(G) = dPI(H) + (d-1)\Big(d(|E(H)|+1)(|E(H)|+1-m_v(H)) - 2\Big),$$

as requested. □

For example, let P_m be the path graph on m vertices $v_1,\ldots,v_m$. Clearly, $PI(P_m) = (m-1)(m-2)$. Let $A_{d,m} := G_d(P_m,v_1)$, see Figure 2 for $m=3$. Clearly, $A_{d,1} = P_m$.

FIGURE 2. The graph $A_{d,3}$

Corollary 2 for $A_{d,m}$ ($m_{v_1}(P_m) = 0$ and $|E(P_m)| = m-1$) gives that

$$PI(A_{d,m}) = d(m-1)(m-2) + (d-1)(dm^2 - 2).$$

Note that one has in particular $A_{2,m} = P_{2m}$, implying $PI(A_{2,m}) = (2m-1)(2m-2)$ which can be checked directly by inserting $d=2$ into the above equation.

As another example, define $T_{d,k} := G_d(C_k,v_1)$, see Figure 3 when $k=3$ and $d=5$.

FIGURE 3. The graph $T_{5,3}$

Corollary 3. *The PI index of $T_{d,k}$ given by*

$$PI(T_{d,k}) = \begin{cases} d^2(k+1)^2 - d(4k+3) + 2, & k \text{ is even}, \\ d^2k(k+1) - 2d(k+1) + 2, & k \text{ is odd}. \end{cases}$$

Proof. Corollary 2 for the bridge graph $T_{d,k}$ gives that

$$PI(T_{d,k}) = dPI(C_k) + (d-1)\Big(d(|E(C_k)|+1)(|E(C_k)|+1-m_v(C_k)) - 2\Big).$$

For k odd one has $PI(C_k) = k(k-1)$ and $m_v(C_k) = 1$, whereas for k even one has $PI(C_k) = k(k-2)$ and $m_v(C_k) = 0$. Inserting these facts yield the asserted equations. □

As another example, define $B_d := G_d(P_3, v_2)$, see Figure 4 (Polyethene when $d = 4$).

FIGURE 4. The graph B_d

Then Corollary 2 for B_d yields that $PI(B_d) = 9d(d-1) + 2$.

As a first step to generalize this result we consider the graphs $B_{d,m;l} := G_d(P_m, v_l)$ where we use a path P_m of arbitrary length m and choose a (fixed) vertex v_l (with $1 \leq l \leq m$) in each P_m. Clearly, $B_{d,3;2} = B_d$ from above. Choosing always the first vertex yields the graph $A_{d,m}$, i.e., $B_{d,m;1} = A_{d,m}$ and, hence, $PI(B_{d,m;1}) = PI(A_{d,m})$. It is easy to check that the PI index of the graph $B_{d,m;l}$ does not depend on the vertex l which we chose in each path (as long as it is the same in each path). Thus, we conclude that

$$PI(B_{d,m;l}) = PI(B_{d,m;1}) = PI(A_{d,m})$$

and the last index has been calculated above. Now, if we want to choose in each path the vertex independently we cannot use directly Corollary 2. However, checking the formula given in Theorem 1 we see that - due to $m_v(P_m) = 0$ for any vertex v in P_m - the resulting formula is the same for any choice of vertices in the paths! Let us describe the result more precisely as follows. Let $\mathcal{I} = (i_1, \ldots, i_d) \in \{1, \ldots, m\}^d$ be a multi-index and denote the bridge graph of d paths P_m joined via the vertices v_{i_k} by $B_{d,m;\mathcal{I}}$, i.e., $B_{d,m;\mathcal{I}} := B(\underbrace{P_m, \ldots, P_m}_{d\ times}; v_{i_1}, v_{i_2}, \ldots, v_{i_d})$. Then the PI index of $B_{d,m;\mathcal{I}}$ is independent of $\mathcal{I}$ and is given by

$$PI(B_{d,m;\mathcal{I}}) = d(m-1)(m-2) + (d-1)(dm^2 - 2).$$

As an example, the graph $B_{3,3;(1,2,1)}$ is displayed in Figure 5.

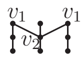

FIGURE 5. The graph $B_{3,3;(1,2,1)}$

4. The chain Graph

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i, w_i \in V(G_i)$, the *chain graph*

$$C(G_1, G_2, \ldots, G_d) = C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$$

of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i, w_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, \ldots, G_d$ by identifying the vertex w_i and the vertex v_{i+1} for all $i = 1, 2, \ldots, d-1$, see Figure 6.

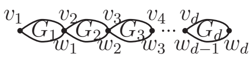

FIGURE 6. The chain graph

In order to compute the PI index of the chain graph $C(G_1, G_2, \ldots, G_d)$ we generalize the notation $M_v(G)$ as follows. Let G be any graph and let $v \in V(G)$ be any vertex of G. For each edge $e = uu' \in E(G)$ we define

$$a_v(e) := \begin{cases} 1, & d(u,v) = d(u',v), \\ 0, & d(u,v) \neq d(u',v). \end{cases}$$

Then for any vertex $w \in V(G)$ such that $w \neq v$, we define $M^{1,1}_{v,w}(G)$ (respectively, $M^{1,0}_{v,w}(G)$, $M^{0,1}_{v,w}(G)$, $M^{0,0}_{v,w}(G)$) to be the set of all edges e in $E(G)$ such that $a_v(e) = a_w(e) = 1$ (respectively, $a_v(e) = 1 - a_w(e) = 1$, $1 - a_v(e) = a_w(e) = 1$, $a_v(e) = a_w(e) = 0$). The cardinality of $M^{s,t}_{v,w}(G)$ is denoted by $m^{s,t}_{v,t}(G)$.

Theorem 4. *The PI index of the chain graph $C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$ is given by*

$$\begin{aligned} PI(G) &= \sum_{j=1}^{d} PI(G_j) + \sum_{j=1}^{d}(|E(G_j)| - m_{w_j}(G_j))(|E(G)| - |E(G_j)|) \\ &\quad + \sum_{j=1}^{d-1} m'_{v_j,w_j}(G_j) \sum_{i=1}^{j-1} |E(G_i)| + (m_{w_d}(G_d) - m_{v_d}(G_d))(|E(G)| - |E(G_d)|) \end{aligned}$$

where $m'_{v_j,w_j}(G_j) := m^{0,1}_{v_j,w_j}(G_j) - m^{1,0}_{v_j,w_j}(G_j)$.

Proof. Let $G = C(G_1, G_2, \ldots, G_d; v_1, w_1, v_2, w_2, \ldots, v_d, w_d)$. From the definitions we have that

$$\begin{aligned} &PI(G) = \sum_{e \in E(G)} n_e(G) = \sum_{i=1}^{d} \sum_{e \in E(G_i)} n_e(G) \\ &= \sum_{e \in E(G_1)} n_e(G) + \sum_{j=2}^{d-1} \sum_{e \in E(G_j)} n_e(G) + \sum_{e \in E(G_d)} n_e(G) \\ &= \sum_{e \in E(G_1) \setminus M_{w_1}(G_1)} n_e(G) + \sum_{e \in M_{w_1}(G_1)} n_e(G) + \sum_{e \in E(G_d) \setminus M_{v_d}(G_d)} n_e(G) + \sum_{e \in M_{v_d}(G_d)} n_e(G) \\ &+ \sum_{j=2}^{d-1} \left(\sum_{e \in M^{0,0}_{v_j,w_j}(G_j)} n_e(G) + \sum_{e \in M^{0,1}_{v_j,w_j}(G_j)} n_e(G) + \sum_{e \in M^{1,0}_{v_j,w_j}(G_j)} n_e(G) + \sum_{e \in M^{1,1}_{v_j,w_j}(G_j)} n_e(G) \right). \end{aligned}$$

Now, let us find each sum in the above expression. In the same fashion as in the proof of Theorem 1 we obtain for the edges in the two graphs G_1 and G_d having only one neighbor that

$$\begin{aligned} \sum_{e \in E(G_1)} n_e(G) &= \sum_{e \in E(G_1) \setminus M_{w_1}(G_1)} n_e(G) + \sum_{e \in M_{w_1}(G_1)} n_e(G) \\ &= \sum_{e \in E(G_1) \setminus M_{w_1}(G_1)} (n_e(G_1) + |E(G)| - |E(G_1)|) + \sum_{e \in M_{w_1}(G_1)} n_e(G_1) \\ &= PI(G_1) + (|E(G_1)| - m_{w_1}(G_1))(|E(G)| - |E(G_1)|), \end{aligned}$$

as well as

$$\begin{aligned}
\sum_{e\in E(G_d)} n_e(G) &= \sum_{e\in E(G_d)\setminus M_{v_d}(G_d)} n_e(G) + \sum_{e\in M_{v_d}(G_d)} n_e(G) \\
&= \sum_{e\in E(G_d)\setminus M_{v_d}(G_d)} (n_e(G_d) + |E(G)| - |E(G_d)|) + \sum_{e\in M_{v_d}(G_d)} n_e(G_d) \\
&= PI(G_d) + (|E(G_d)| - m_{v_d}(G_d))(|E(G)| - |E(G_d)|).
\end{aligned}$$

The contributions for the edges contained in one of the graphs G_j $(2 \leq j \leq d-1)$ having two neighbors are given by the following formulas:

$$\begin{aligned}
\sum_{e\in M^{0,0}_{v_j,w_j}(G_j)} n_e(G) &= \sum_{e\in M^{0,0}_{v_j,w_j}(G_j)} (n_e(G_j) + |E(G)| - |E(G_j)|), \\
\sum_{e\in M^{0,1}_{v_j,w_j}(G_j)} n_e(G) &= \sum_{e\in M^{0,1}_{v_j,w_j}(G_j)} (n_e(G_j) + |E(G_1)| + \cdots + |E(G_{j-1})|), \\
\sum_{e\in M^{1,0}_{v_j,w_j}(G_j)} n_e(G) &= \sum_{e\in M^{1,0}_{v_j,w_j}(G_j)} (n_e(G_j) + |E(G_{j+1})| + \cdots + |E(G_d)|), \\
\sum_{e\in M^{1,1}_{v_j,w_j}(G_j)} n_e(G) &= \sum_{e\in M^{1,1}_{v_j,w_j}(G_j)} n_e(G_j).
\end{aligned}$$

Adding the above contributions yields for j such that $2 \leq j \leq d-1$ that

$$\begin{aligned}
&\sum_{e\in E(G_j)} n_e(G) \\
&= PI(G_j) + m^{0,0}_{v_j,w_j}(G_j)(|E(G)| - |E(G_j)|) + m^{0,1}_{v_j,w_j}(G_j)(|E(G_1)| + \cdots + |E(G_{j-1})|) \\
&\quad + m^{1,0}_{v_j,w_j}(G_j)(|E(G_{j+1})| + \cdots + |E(G_d)|), \\
&= PI(G_j) + m^{0,0}_{v_j,w_j}(G_j)(|E(G)| - |E(G_j)|) + m^{0,1}_{v_j,w_j}(G_j)(|E(G_1)| + \cdots + |E(G_{j-1})|) \\
&\quad + m^{1,0}_{v_j,w_j}(G_j)(|E(G)| - |E(G_1)| - \cdots - |E(G_j)|), \\
&= PI(G_j) + (m^{0,0}_{v_j,w_j}(G_j) + m^{1,0}_{v_j,w_j}(G_j))(|E(G)| - |E(G_j)|) \\
&\quad + (m^{0,1}_{v_j,w_j}(G_j) - m^{1,0}_{v_j,w_j}(G_j))(|E(G_1)| + \cdots + |E(G_{j-1})|).
\end{aligned}$$

Using

$$\begin{aligned}
m^{0,0}_{v_j,w_j}(G_j) + m^{1,0}_{v_j,w_j}(G_j) &= |E(G_j)| - m^{1,1}_{v_j,w_j}(G_j) - m^{0,1}_{v_j,w_j}(G_j) \\
&= |E(G_j)| - m_{w_j}(G_j),
\end{aligned}$$

we obtain that the PI index of the graph G is given by

$$\begin{aligned} PI(G) &= \sum_{j=1}^{d} PI(G_j) + \sum_{j=1}^{d} (|E(G_j)| - m_{w_j}(G_j))(|E(G)| - |E(G_j)|) \\ &+ \sum_{j=2}^{d-1} m'_{v_j,w_j}(G_j) \sum_{i=1}^{j-1} |E(G_i)| + (m_{w_d}(G_d) - m_{v_d}(G_d))(|E(G)| - |E(G_d)|), \end{aligned}$$

completing the proof. □

Define $T_d(H, v, w) := C(\underbrace{H, H, \ldots, H}_{d \text{ times}}, \underbrace{v, w, v, w, \ldots, v, w}_{d \text{ times}})$. As a corollary of Theorem 4 we have the following result.

Corollary 5. *The PI index of the graph $T_d(H, v, w)$ is given by*

$$\begin{aligned} &PI(T_d(H, v, w)) \\ &\quad = dPI(H) + (d-1)|E(H)| \left\{ d(|E(H)| - m_w(H)) + \tfrac{(d-2)}{2} m'_{v,w}(H) + m''_{v,w}(H) \right\} \end{aligned}$$

where $m'_{v,w}(H) := m^{0,1}_{v,w}(H) - m^{1,0}_{v,w}(H)$ and $m''_{v,w}(H) := m_w(H) - m_v(H)$.

For example, if SL_d is the following graph, then Corollary 5 for H a square (here

FIGURE 7. The graph SL_d

$m^{0,1}_{v,w}(H) = m^{1,0}_{v,w}(H) = m_w(H) = m_v(H) = 0$ and $PI(H) = 8$) gives that the PI index of SL_d is given by $PI(SL_d) = 8d(2d-1)$.

Let H be any graph with fixed two vertices v, w and let P_2 be a graph of one edge connecting the two vertices v', w'. Define

$$U_d(H) := C(H, P_2, \ldots, H, P_2, H, v, w, v', w', \ldots, v, w, v', w', v, w)$$

(d copies of H) as described in Figure 8.

As a corollary of Theorem 4 we have the following result.

FIGURE 8. The chain graph $U_d(H)$

Corollary 6. *The PI index of the graph $U_d(H)$ is given by*

$$\begin{aligned} &PI(U_d(H)) \\ &= dPI(H) \\ &\quad +(d-1)\Big\{|E(H)|\{d(|E(H)|-m_w(H))+m''_{v,w}(H)+\tfrac{(d-2)}{2}m'_{v,w}(H)+d\} \\ &\quad +d(|E(H)|-m_w(H))+m''_{v,w}(H)+d-2\Big\} \end{aligned}$$

where $m'_{v,w}(H) = m^{0,1}_{v,w}(H) - m^{1,0}_{v,w}(H)$ and $m''_{v,w}(H) = m_w(H) - m_v(H)$.

Example 7 (Polyphenylenes)**.** *Consider the chain graph $U_d(H)$ where H is a hexagon with vertices $v_1, v_2, v_3, v_4, v_5, v_6$ (labelled clockwise), $v = v_1$ and $w = v_4$. From the definitions we have that $|E(H)| = 6$, $m'_{v,w}(H) = m_v(H) = m_w(H) = 0$ and $PI(H) = 24$. Then Corollary 6 gives*

$$PI(U_d(H)) = 24d + (d-1)\{6(6d+d)+6d+d-2\} = 49d^2 - 27d + 2,$$

as shown in [14].

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