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On edge Co-PI indices

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Abstract

In this paper, at first we mention to some results related to PI and vertex Co-PI indices and then we introduce the edge versions of Co-PI indices. Then, we obtain some properties about these new indices.

Keywords : Vertex-PI index- Edge-PI indices; Molecular graph; Vertex Co-PI indices.

1 Introduction

IN the fields of chemical graph theory and in mathematical chemistry, a topological index, also known as a connectivity index, is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound [17]. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure [6].

Let G be a simple molecular graph without directed and multiple edges and without loops. The graph G consists of the set of vertices $V(G)$ and the set of edges$E(G)$. In molecular graph, each vertex represented an atom of the molecule and bonds between atoms are represented by edges between corresponding vertices.

Khadikar and Co-authors in [12, 13, 14, 15] defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. If $e = uv$ is an edge of G, it is defined as

$$PI_e(G) = \sum_{e\in E(G)} [m_e(u) + m_e(v)] \tag{1.1}$$

where $m_e(u)$ is the number of edges of G lying closer to u than to v and $m_e(v)$ is

The distance between to vertices $x, y \in V(G)$ is equal to the number of edges on shortest path between them and it is shown by $d(x, y)$.

Now, according to distance between vertices, we can restate $m_e(u)$ and $m_e(v)$as follow:

$$m_e(u) = |A| = \left|\left\{f \in E(G)\,\middle|\,d'(f,u) < d'(f,v)\right\}\right|$$

$$m_e(v) = |B| = \left|\left\{f \in E(G)\,\middle|\,d'(f,v) < d'(f,u)\right\}\right|$$

where $d'(f, u) = \min\{d(x, u), d(y, u)\}$ such that $f = xy \in E(G)$ and $u \in V(G)$.

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This is the first-edge version of PI index and in [2, 3, 4] and [8, 9, 10], the edge-PI index has been computed for some graphs.
This version of PI index can be restated in following the formula.

$$PI_e(G) = \sum_{e\in E(G)} (|E(G)| - m(e)) \qquad (1.2)$$

where $m(e)$ is the number of edges which have equal to distance from u and v.
The vertex version of PI index was also defined in [18], as follows:

$$PI_v(G) = \sum_{e\in E(G)} [n_e(u) + n_e(v)] \qquad (1.3)$$

where
$n_e(u) = |C| = |\{x \in V(G)\,|d(x,u) < d(x,v)\,\}|$
and
$n_e(v) = |D| = |\{x \in V(G)\,|d(x,v) < d(x,u)\,\}|$.
And we can restate it as follow:

$$PI_v(G) = \sum_{e\in E(G)} (|V(G)| - n(e)) \qquad (1.4)$$

where $n(e)$ the number of edges which have equal to distance from u and v. You can find some computations in [16].
The second edge version of PI index was introduced recently in [11], as follow:

$$PI'_e(G) = \sum_{e\in E(G)} [m'_e(u) + m'_e(v)] \qquad (1.5)$$

where
$m'_e(u) = |E| = |\{f \in E(G)\,|d'''(f,u) < d'''(f,v)\,\}|$ and
$m'_e(v) = |F| = |\{f \in E(G)\,|d'''(f,v) < d'''(f,u)\,\}|$.
Also, d''' is:

$$d'''(f,u) = \begin{cases} d''(f,u) & ,u \notin f \\ 0 & ,u \in f \end{cases}$$

where if $f = xy \in E(G)$ and $u \in V(G)$, then $d''(f,u) = \max\{d(x,u), d(y,u)\}$.
This version can restate as follow, too:

$$PI'_e(G) = \sum_{e\in E(G)} \big(|E(G)| - m'(e)\big) \qquad (1.6)$$

where $m'(e)$ is the number of edges which have equal to distance from u and v according to d'''.
Iranmanesh et. al. introduced the new index similar to the vertex version of PI index recently [7].
This index is named the first vertex Co-PI index which is

$$Co - PI_v(G) = \sum_{e\in E(G)} |n_e(u) - n_e(v)|\,.$$

In [1], the first vertex Co-PI index is restated to

$$co{-}PI_v(G) = \sum_{uv=e\in E(G)} \left|\sum_{x\in V(G)} (d(u,x) - d(v,x))\right|$$

Recently, the second vertex version of Co-PI index introduced in [1] as follows

$$co{-}PI'_v(G) = \sum_{x\in V(G)} \left|\sum_{uv=e\in E(G)} (d(u,x) - d(v,x))\right|$$

In this paper, at first we mention to some results related to PI and vertex Co-PI indices and then we introduce the edge versions of Co-PI index with the name of edge Co-PI indices. Then, we obtain some properties about these new indices.

2 Discussion and results

A useful relation concerning distances of two vertices which are adjacent stated in [5].

Lemma 2.1 *[5] Suppose $x, y \in V(G)$ are two adjacent vertices of a connected graph G and suppose $xy = e \in E(G)$. Then $d(x) - d(y) = n_e(y) - n_e(x)$ where $d(x) = \sum_{y\in V(G)} d(x,y)$.*

This property gives us several ideas about PI indices for example: restating the edge PI indices according to distances and defining the new indices similar to edge PI indices.

Theorem 2.1 *Let G be a connected graph. Then*
I) $PI_e(G) = \sum_{e\in E(G)} \sum_{f\in E(G)} |d'(u,f) - d'(v,f)|$
II) $PI'_e(G) = \sum_{e\in E(G)} \sum_{f\in E(G)} |d'''(u,f) - d'''(v,f)|$

Proof. For the proof of the above formulas, they are:
Suppose $uv = e \in E(G)$. Then

i) $m_e(u) + m_e(v) = \sum_{f\in E(G)} |d'(u,f) - d'(v,f)|$
ii) $m'_e(u) + m'_e(v) = \sum_{f\in E(G)} |d'''(u,f) - d'''(v,f)|$

We can obtain easily the Relations (I, II) from the Relations (i, ii) and (1.3 and 1.5).
Now, we prove only the Relation (i) and the proof of other Relation (ii) is similar to the proof of Relation (i).
Let $uv = e \in E(G)$, then for each $f \in E(G)$, we have

$$\left|d'(u,f) - d'(v,f)\right| = \begin{cases} 1 & , f \notin m(e) \\ 0 & , f \in m(e) \end{cases}$$

Therefore, $\sum_{f\in E(G)} |d'(u,f) - d'(v,f)| = E(G) - m(e) = m_e(u) + m_e(v)$. $\square$
Now, we want to introduce the edge versions of Co-PI indices.

Definition 2.1 *The Co-PI indices are:*

1. $Co - PI_e(G) = \sum_{e\in E(G)} |m_e(u) - m_e(v)|$
2. $Co - PI'_e(G) = \sum_{e\in E(G)} |m'_e(u) - m'_e(v)|$

We name the Relation (a) as first edge Co-PI index and Relation (b) as second edge Co-PI index.
In following theorem, we restate the edge Co-PI indices.

Theorem 2.2 *The edge Co-PI indices according to distances are:*
III) $Co - PI_e(G) = \sum_{e\in E(G)} \left|\sum_{f\in E(G)} (d'(u,f) - d'(v,f))\right|$
IV) $Co - PI'_e(G) = \sum_{e\in E(G)} \left|\sum_{f\in E(G)} (d'''(u,f) - d'''(v,f))\right|$

Proof. It is sufficient we prove the following relations for obtain the Relations (III, IV). Suppose $uv = e \in E(G)$. Then
iii) $m_e(u) - m_e(v) = \sum_{f\in E(G)} d'(v,f) - d'(u,f)$
iv) $m'_e(u) - m'_e(v) = \sum_{f\in E(G)} d'''(v,f) - d'''(u,f)$
We can obtain easily the Relations (III and IV) from the Relations (iii and iv) and (1 and 2).
Now, we prove only the Relation (iii) and the proof of other Relation (iv) is similar to the proof of Relation (iii).
Let $uv = e \in E(G)$, then for each $f \in E(G)$, we have

$$d'(v,f) - d'(u,f) = \begin{cases} 1 & , \quad f \in C \\ 0 & , \quad f \in n(e) \\ -1 & , \quad f \in D \end{cases}$$

Therefore, $\sum_{f\in E(G)} d'(v,f) - d'(u,f) = m_e(u) - m_e(v)$. (The relation (iv) can be obtained from (Lemma 2.1, too.) $\square$
In next part, we compute the co-PI indices for some graph.

3 Computations

At first, we compute the edge Co-PI indices for cycles and we conclude that there is only one edge Co-Pi indices. Next, we compute the second vertex co-PI index for some 2-colorable graphs.

Lemma 3.1 *Let G be the cycle C_n. Then, $co - PI_e(G) = 0$ and $co - PI'_e(G) = 0$.*

Proof. Let G be C_n. In graph G if n is even or odd, then $m_e(u) = m_e(v)$ and $m'_e(u) = m'_e(v)$. Therefore, $co - PI_e(G) = 0$, $co - PI'_e(G) = 0$.$\square$
At following, we conclude an interesting result about edge versions of co-PI index.

Theorem 3.1 *The first edge co-PI index is equal to the second edge co-PI index i.e. $co - PI_e(G) = co - PI'_e(G)$ for each graph G.*

Proof. In Ref. [10], it is proved that $PI_e(G) \geq PI'_e(G)$ for arbitrary graph G. Also, it is proved $PI_e(G) = PI'_e(G)$ and in particular $m_e(u)= m'_e(u)$ and $m_e(v)= m'_e(v)$ for each graph without odd cycles. The difference between $m_e(u)$ and $m'_e(u)$ ($m_e(v)$ and $m'_e(v)$) is the result of existing of odd cycles in graphs and this difference is $m_e(u) - m'_e(u) = O(G) = m_e(v) - m'_e(v)$ which $O(G)$ is the number of odd cycles in graph G. Therefore, we have for edges of odd cycles in graph G $m_e(u) - m_e(v) = m'_e(u) - m'_e(v)$. Then, for each edge of graph G, we have $m_e(u) - m_e(v) = m'_e(u) - m'_e(v)$. Hence, $co - PI_e(G) = co - PI'_e(G)$.$\square$
Due to Theorem (3.2), there is only one edge co-PI index. This result is important result about edge version of co-PI index.

Table 1: The different versions of co-PI index for some well known graphs.

G	$co-PI_v(G)$	$co-PI'_v(G)$	$co-PI_e(G)$
S_n	$(n-1)(n-2)$	-	$(n-1)(n-2)$
K_n	0	-	0
$K_{a,b}$	$ab\,\lvert a-b\rvert$	$a\,\lvert ab-2(b)\rvert+b\,\lvert ab-2(a)\rvert$	$ab\,\lvert a-b\rvert$

There is an easy result about 2-colorable graphs that we bring it as lemma without proof.

Lemma 3.2 *Let G be a graph. Then, G is 2-colorable iff G is bipartite graph.*

Therefore, we have:

Theorem 3.2 *The second vertex co-PI index for some bipartite graphs are as follows:*

1. *Let $K_{a,b}$ be the complete bipartite graph. Then,*

$$co-PI'_v(K_{a,b}) = a\,|ab-2(b)|+b\,|ab-2(a)|\,.$$

2. *Let $L_{h,i}$ be a linear chain with h ring which each ring contains i edges and $i$is the even numbers $i = 4, 6, 8, \ldots$. Then,*

$$co-PI'_v(L_{h,i}) =$$

$$\begin{cases} (2kh+1)\left(|h-3|+|h+1|\right) & , i = 4k+2 \\ (8k-4)h+4 & , i = 4k \end{cases}$$

where $k \in \mathrm{N} = \{1, 2, 3, 4, \ldots\}$.

Proof. In ref. [10] Let $K_{a,b}$ be the complete bipartite graph. Give the label $u$for $a$vertices which are in a part and label v for $b$vertices in other part. At first, fix a vertex with label u. Then

$$\sum_{xy=e\in E(k_{a,b})} (d(u,x)-d(u,y)) =$$

$$(-1)b+(1)(ab-b) = ab-2b$$

Now, fix a vertex with label v. Then

$$\sum_{xy=e\in E(k_{a,b})} (d(v,x)-d(v,y)) =$$

$$(1)a+(-1)(ab-a) = -ab+2a$$

Therefore,

$$co-PI'_v(K_{a,b}) = a\,|ab-2(b)|+b\,|ab-2(a)|\,.$$

(1.2). Let $L_{h,i}$ be a linear chain with h ring which each ring contains i edges ($i = 4, 6, 8, \ldots$). The number of vertices and edges of chain are $ih-2h+2$ and $ih-h+1$, respectively. For example see the linear chains $L_{3,6}$ and $L_{3,4}$ in Figure 1 with labels u and v. We denote the outer cycle of $L_{h,i}$ with Cwhich has $ih-2h+2$ edges and the set of common edges between rings with Swhich has $h-1$elements.

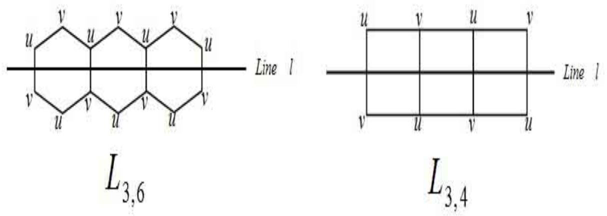

Figure 1

Because of the labels of edges elements of S, we divide the set $\{4, 6, 8, \ldots\}$ to two subsets $\{4, 8, 12, \ldots\}$ and $\{6, 10, 14, \ldots\}$. Therefore:

1. Suppose $i = 4k+2$ which $k = 1, 2, 3, \ldots$ and fix a vertex with label u in top of line l. Therefore, $\sum_{xy=e\in C}(d(u,x)-d(u,y)) = -2$ and $\sum_{xy=e\in S}(d(u,x)-d(u,y)) = -(h-1)$.

fix a vertex with label u in below of line l. Therefore, $\sum_{xy=e\in C}(d(u,x)-d(u,y)) = -2$ and $\sum_{xy=e\in S}(d(u,x)-d(u,y)) = (h-1)$.
And we do the same procedure for vertices with label v. Hence, $co-PI'_v(L_{h,i}) = \frac{|V(L_{h,i})|}{2}\,|h+1| + \frac{|V(L_{h,i})|}{2}\,|h-3|$.

1. Suppose $i = 4k$ which $k = 1, 2, 3, \ldots$ and fix a vertex with label u in top of line l. Therefore, $\sum_{xy=e\in C}(d(u,x)-d(u,y)) = -2$

and $\sum_{xy=e\in S}(d(u,x)-d(u,y)) = \begin{cases} 0 & ,h \ \ is \ \ odd \\ 1 & ,h \ \ is \ \ even \end{cases}.$

fix a vertex with label u in below of line l. Therefore, $\sum_{xy=e\in C}(d(u,x)-d(u,y)) = -2$ and $\sum_{xy=e\in S}(d(u,x)-d(u,y)) = \begin{cases} 0 & ,h \ \ is \ \ odd \\ -1 & ,h \ \ is \ \ even \end{cases}.$
And we do the same procedure for vertices with label v. Hence, $co-PI'_v(L_{h,i}) = 2\,|V(L_{h,i})|$.
Therefore,

$$co-PI'_v(L_{h,i}) =$$

$$\begin{cases} (2kh+1)\left(|h-3|+|h+1|\right) & ,i=4k+2 \\ (8k-4)h+4 & ,i=4k \end{cases}.$$

□

Now, we compute the vertex versions and edge version of co-PI index for some familiar graphs that the results of computations are shown in Table 1.

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