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Research Article

COMPUTING NEW VERSION OF PI INDEX FOR ROOTED GRAPHS

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ABSTRACT
In mathematics and in particular in graph theory, a rooted graph is a graph in which one vertex has been distinguished as the root. Also, for an edge e=*ab* of a graph *G*, *let* W_{ab}^G be the set of vertices closer to *a* than to *b*. That is

$$W_{ab}^G = \{u \in V(G) \mid d(u,a) < d(u,b)\}$$

We call a graph *G distance-balanced*, if $|W_{ab}^G| = |W_{ba}^G|$ holds for any edge *ab* of *G*. In this paper, some properties of rooted and distance balanced graphs about new version of PI index is computed.

Keywords: *Rooted Graph, Molecular Graphs, Distance-balanced Graph, New Version of PI Index*

INTRODUCTION
In the fields of chemical graph theory, molecular topology, and 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 (Hendrik *et al.,* 2002). 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 (Hall *et al.*, 1976).

Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices (e.g., distance or adjacency matrices), which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index (González-Díaz *et al.,* 2007; González-Díaz *et al.,* 2008). As a result, the topological index can be defined as two-dimensional descriptors that can be easily calculated from the molecular graphs, and do not depend on the way the graph is depicted or labeled and no need of energy minimization of the chemical structure.

The simplest topological indices do not recognize double bonds and atom types (C, N, O, etc.) and ignore hydrogen atoms ("hydrogen suppressed") and defined for connected undirected molecular graphs only (King, 1983). More sophisticated topological indices also take into account the hybridization state of each of the atoms contained in the molecule. Hundreds of indices were introduced. The Hosoya index is the first topological index recognized in chemical graph theory, and it is often referred to as the topological index (Hosoya, 1971). Other examples include the Wiener index, Randić's molecular connectivity index, Balaban's J index (Katritzky *et al.,* 2002), and the TAU descriptors (Pal *et al.,* 1988; Pal *et al.,* 1989). The extended topochemical atom (ETA) indices have been developed based on refinement of TAU descriptors (Roy *et al.,* 2003).

Global and Local Indices
Wiener index are global (integral) indices to describe entire molecule, Bonchev and Polansky introduced local (differential) index for every atom in a molecule (Hosoya, 1971). Since then Wiener index is widely used in QSPR/QSAR/QSTR studies. This index is defined as below:

$$W(G)=\Sigma d(i, j), \quad (1)$$

where d(i, j) is the size of minimum length of paths between vertices i and j.

The *Wiener index* W = W(G) was first defined for a tree G = T by the following expression:

$W = W(T) = (1/2)\Sigma d(i, j)$, (2)
where the summation going over all pairs (i, j) of vertices i, j∈V (G), or by
$W = W(T) = \Sigma n_i(e)\, n_j(e)$, (3)
where the summation going over all edges e = (i, j) ∈ E (G).
The Szeged index Sz (G) of graph G is defined (see also equations (1), (2)) by
$Sz(G) = \Sigma n_i(e)\, n_j(e)$. (4)
The right-hand side of eq. (4), although formally identical to the right-hand side of eq. (3), differs in the interpretation of $n_i(e)$ and n(j(e)). In the former case, eq. (3), they are the number of vertices of G lying on two sides of the edge e. While in case of eq. (4), if we define an edge e = uv, then $n_i(e)$ is the number of vertices closer to u than v, and $n_j(e))$ is the number of vertices closer to v than u; vertices equidistant to u and v are not counted. For more details please see (Diudea *et al.,* 2006).
Since Sz and W indices of acyclic graphs coincide, Khadikar to remove this lacuna, proposed another index in 2000, which he named Padmakar-Ivan index and abbreviated as PI (Khadikar *et al.,* 2000; Khadikar *et al.,* 2001). It is worth mentioning that Padmakar is the first name of Khadikar, while Ivan is the first name of Gutman. Khadikar conceived this index while attempting simultaneous estimation of Wiener and Szeged indices of benzenoids using elementary cut method. The Padmakar-Ivan index (abbreviated as PI index) of a molecular graph is defined by the following expression:
$PI = PI(G) = \Sigma_{e\in E(G)} [n_{eu}(e \mid G) + n_{ev}(e \mid G)]$.
Here, we define edge of G connecting the vertices u and v, as e = *uv* ∈ E (G). The quantities n_{eu} and n_{ev} are the number of edges closer to u and v respectively. In calculating PI index edges equidistance from both end of the edge *uv* are not counted. The PI index of acyclic and cyclic graphs differs.
After the PI index, Hasani *et al.,* (2010) difined the new index similar to the vertex version of PI index abbreviated CO-PI index (Hasani *et al.,* 2010). This index is defined as:

$$CO-PI(G)=\sum_{e=uv\in E(G)} |n_e(u)|-|n_e(v)|$$

Through this paper, some properties about CO-PI index of molecular graphs is included. Our notation is standard and is similar to Handbook of Molecular Descriptors (Hendrik *et al.,* 2002).

RESULTS AND DISCUSSION

In this section we will use some definitions and theorem from Hall *et al.,* (1976) to calculate the Co- PI index of graphs.

Definition. Rooted graph: In mathematics and in particular in graph theory, a rooted graph is a graph in which one vertex has been distinguished as the root.
Both directed and undirected versions of rooted graphs have been studied, and there are also variant definitions that allow multiple roots.

Definition. Distance-balanced graph: For an edge e= *ab* of a graph *G*, *let* W_{ab}^G be the set of vertices closer to *a than* to *b*. That is

$$W_{ab}^G = \{u\in V(G) \mid d(u,a) < d(u,b)\}$$

We call a graph *G distance-balanced*, if $|W_{ab}^G| = |W_{ba}^G|$ holds for any edge *ab* of *G*.

Definition. Suppose that *G* and *H* are graphs with disjoint vertex sets. Following Doslic (Doslic, (2008)), for given vertices $y \in V(G)$ and $z \in V(H)$ a splice of *G* and *H* by vertices *y* and *z*, $(G \cdot H)(y; z)$, is defined by identifying the vertices *y* and *z* in the union of *G* and *H*. Similarly, a link of *G* and *H* by vertices *y* and *z* is defined as the graph $(G \circ H)(y; z)$ obtained by joining *y* and *z* by an edge in the union of these graphs.
In the following proposition, the Co-PI index for rooted and distance balanced graph $(G \cdot H)(a; b)$ is computed.

Proposition. Assume that G and H are rooted graphs with respect to the rooted vertices of a and b, respectively. Also (G · H)(a; b) is distance-balanced. Then the Co-PI index of graphs G and H are equal to:
Co-PI (G) = (| V(H)| -1). |A| and Co-PI (H) = (| V(G)| -1). |B|, where, for each arbitrary e = uv ∈ E(G) and f = xy ∈ E(H), A, B are equal to this following sets:
A = {e = uv ∈ (G · H)(a; b)|d(v; a) < d(u; a)};
B = {e = uv ∈ (G · H)(a; b)|d(v; r) = d(u; r)}:
Proof . Suppose that r = a = b. We partition edges of (G·H)(a; b) into the following two subsets:
A = {e = uv ∈ E(G:H)|d(v; r) < d(u; r)};
B = {e = uv ∈ E(G:H)|d(v; r) = d(u; r)}.
Since G and H are rooted graphs with respect to the rooted vertices of a and b, respectively, and (G · H)(a; b) is distance-balanced**,** thus by Tavakoli**,** Proposition 2.3 (Tavakoli *et al.*, 2013), it is obvious that:

$$n_u^G(e) - n_v^G(e) = \begin{cases} |V(H)| - 1, & if \ d(v,a) < d(u,a) \\ 0, & if \ d(v,a) = d(u,a) \end{cases}$$

and

$$n_x^H(e) - n_y^H(e) = \begin{cases} |V(G)| - 1, & if \ d(y,b) < d(x,b) \\ 0, & if \ d(y,b) = d(x,b) \end{cases}$$

Therefore, by diofinition of Co-PI index, we have, Co-PI index of graphs G and H are equal to:
Co-PI (G) = (| V(H)| -1). |A| and Co-PI (H) = (| V(G)| -1). |B|.

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