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Research Article

COMPUTING CO-PI INDEX OF EDGE DISTANCE-BALANCED GRAPHS

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ABSTRACT
Let G be a graph and e = uv ∈E(G), m^G_u (e) denotes the number of edges lying closer to the vertex u than the vertex v, and m^G_v (e) is defined analogously. Here is our key definition. We call a graph G to be edge distance-balanced, if m^G_a (e) = m^G_b (e) holds for each edge e = ab ∈ E (G). In this paper, most important topological index called "CO-PI" of some edge distance-balanced graphs is computed for first time.

Keywords: *Co-PI Index, Chemical Graph, Edge Distance-Balanced Graph, Rooted Graph*

INTRODUCTION

A topological index is a numerical quantity derived in an unambiguous manner from the structural graph of a molecule (Agrawal, 2001; Estrada *et al.*, 1988; Gravac *et al.*, 1977; Gutman, 1977; Hosoya *et al.*, 1976; Madan, 1997; Qian *et al.*, 2003; Gutman *et al.*, 1986). It is a number extracted by a well defined algorithm from a graphical representation of a molecule.

There is good reason to believe that often our difficulties in attributing a meaning to this number lie under deeper chemical theories and higher level languages and not from esoteric approaches to its definition. These indices are graph invariants which usually reflect molecular size, shape, branching, and heterogeneity (Wiener, 1947; Diudea *et al.*, 1997, 1998, 1995, 2000).

Wiener originally defined his index (W) on trees and studied its use for correlations of physicochemical properties of alkanes, alcohols, amines, and their analogous compounds (Wiener, 1947).

The original definition of Wiener index (W) was given in terms of edge weights. In an arbitrary tree, every edge is a bridge, that is, after deletion of the edge; the graph is no more connected (Klein *et al.*, 1995).

The weight of an edge is taken to be the product of the number of vertices in the two connected components. This number also equals the number of all shortest paths in the tree, which go through the edge. Therefore, the usual generalization to the Wiener Index (W) on arbitrary graphs is defined to be the same of all distances in a graph.

Another natural generalization was previously put forward by Gutman and called the Szeged index, abbreviated as Sz. Now, the weights of edges are taken to be the product of the numbers of vertices closed to the two ends of the edge. For reasons to introduce Szeged index, and for its basic properties, uses see reference (Gutman, 1980; Gutman *et al.*, 1997).

For the reason of the coincidence of Wiener and Szeged indices in case of trees (acyclic graphs), we have very recently introduced another Szeged / Wiener-like topological index and named it Padmakar-Ivan index, and abbreviated as PI.

See: (Erovnic, 1999; Khadikar *et al.*, 1995; Chan *et al.*, 1998; Christian *et al.*, 1999; David 2000; Devillers, 1999, 1997).

Unlike Szeged index (Sz), PI index is different for trees as well as for cyclic graphs, and not much is known about the applicability of PI index in chemistry.

Apart from the Wiener index, there are numerous indices associated to a graph which are invariant under the automorphism group of the graph. Another topological index that we are interested in is called the CO-PI index and is defined as follows (Hassani *et al.*, 2010).

Let $G = (V; E)$ be a simple connected graph and $e = uv$ be anedge in E. By $m_u{}^G(e)$ we mean the number of edge in $E(G)$ lying closer to u than v. The quantity $m_v{}^G(e)$ is defined similarly.

The CO-PI index of the graph $G = (V; E)$ is defined by the formula:

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$$\text{CO-PI(G)} = \sum_{e=uv\in G\{H\}} (m_u^G(e) - m_v^G(e))$$

In this paper, we compute Co-PI index of some graphs called "distance balanced". Through this paper, our notation is standard and similar to graph theory and chemical graph theory books (Gutman *et al.*, 1991; Harary, 1969; Trianjestic, 1992).

Definition of Some Topological Indices

In this section we define some graph matrices and some topological indices.
In table 1, we define some graph matrices which applied in computing some topological indices.

Table 1: Graph matrices

Name of matrix (reference)	Definition
The Adjacency Matrix (Lukovits, 2000)	$[A]_{ij} = 1$ if $i \neq j$ and $eij \in E(G)$ $= 0$ if $i = j$ or $e_{ij} \notin E(G)$
Distance matrix (Rouvary, 1986; Mihalic *et al.*, 1992; Bonchev and Tinajstic, 1977)	$[D]_{ij} = \min(l(p_{ij}))$ if $i \neq j$, $= 0$ if $i = j$, D=D(G) where $\min(l(p_{ij}))$ is the length of shortest path between vertices(atoms) i and j.
Reciprocal matrix (Ivanciuc, 1989; Plavsic *et al.*, 1993; Ivanciuc *et al.*, 1993; Amic *et al.*, 1991)	$[RD]_{ij} = 1/D_{ij}$ if $i \neq j$ $= 0$ if $i = j$, RD=RD(G) in which, the elements of RD is the reciprocal (excluding the zero elements) of the elements of D matrix.

There have been more than 400 kinds of topological indices available, since the birth of the first one. Topological index can be used to evaluate structural similarity and diversity. Its main role is to work as a numerical molecular descriptor in QSAR/QSPR model (Ivanciuc *et al.*, 1999; Medic *et al.*, 1992; Balaban *et al.*, 1990, 1986, 1995, 1998, 1992; Ivanciuc *et al.*, 1999; Basak *et al.*, 1994, 1999; Bonchev, 1997, 2000, 2001, 1994, 1977; Barys *et al.*, 1983; Geiss *et al.*, 2001; Estrada, 1998, 1988). Some important indices are listed in Table 2.

Table 2: Topological Index of Molecular Structure

Topological Index of Molecular Structure	
Name of index (reference)	**Definition**
Balaban index J (Balaban, 1982)	$= \Sigma(S_i\ S_j)^{-1/2} = q\Sigma(S_iSj)^{-1/2}$, where Si and Sj mean the distance sums of the vertices V_i and V_j; $q = n_e/(\mu + 1)$, in which $_{ne}$ is the number of edges and μ is the cycle number.
Detour index (Lukovits, 1996; Razinger, 1997)	$\omega = (1/2)\ \Sigma(\Delta)_{ij}$, where Δ_{ij} is an element in the detour matrix.
Harary index (Plavsic *et al.*, 1993)	$H = (1/2)\ \Sigma_i\Sigma_j i=1(D_r)_{ij}$
Hosoya index (Hosoya, 1971)	$Z(G) = \sum_{k=0}^{n/2} P(G,K)$, where $p(G,K)$ is the number of ways in which k edges of the graph may be chosen so that no two of them are adjacent.
Hyper-Wiener index (Klein *et al.*, 1995)	$WW(G) = 1/2 \sum_{i,j} ([D]^2_{ij} + [D]_{ij})$.

Szeged index (Khadikar *et al.*, 1995)	$Sz(G) = \sum_{e=uv \in E(G)} N_u(e\|G) N_v(e\|G)$ Where, $N_u(e\|G)$ is the number of vertices of G lying closer to u and $N_v(e\|G)$ is the number of vertices of G lying closer to v.
Padmakar-Ivan(PI) index (Khadikar *et al.*, 1997)	$PI(G) = \|E(G)\|^2 - \sum_{e \in E(G)} N(e)$ $N(e) = \|E(G)\| - \sum (n_{eu}(e\|G) + n_{ev}(e\|G))$. in which, $m_u^G(e)$ is the number of edge in *E(G)* lying closer to *u* than *v*, fore every arbitrary edge e=uv in E(G). The quantity $m_v^G(e)$ is defined similarly
Molecular topological index (Schultz, 1989)	$MTI = \Sigma E_i$, in which E_i is the row matrix consisting of v(A+D) where v is the vertex degree.
CO-PI index (Hassani *et al.*, 2012)	$CO\text{-}PI(G) = \sum_{e=uv \in G\{H\}} (m_u^G(e) - m_v^G(e)$ in which, $m_u^G(e)$ is the number of edge in *E(G)* lying closer to *u* than *v*, fore every arbitrary edge e=uv in E(G). The quantity $m_v^G(e)$ is defined similarly.

RESULTS AND DISCUSSION

We begin this section with some definition of Vertex and Edge distance-balanced graph. In this section we will use some definitions and theorem from Hall *et al.*, (1976) to calculate the Co- PI index of some graphs.

Definition. **Vertex and Edge distance-balanced graph:**

A connected graph G is said to be distance-balanced whenever for any pair of adjacent vertices u, v of G the number of vertices closer to u than to v is equal to the number of vertices closer to v than to u.

In the other hand, a graph G is said to be distance-balanced, if $n^G{}_a(e) = n^G{}_b(e)$, for each edge $e = ab \in E(G)$, see (Ili'c *et al.*, 2010), for details. These graphs were, at least implicitly, first studied by Handa (1999) who is considered distance-balanced partial cubes. The term itself, however, is due to Jerebific *et al.*, (2008) who is studied distance-balanced graphs in the framework of various kinds of graph products. Let G be a graph, $e = uv \in E(G)$, $m^G{}_u(e)$ denotes the number of edges lying closer to the vertex u than the vertex v, and $m^G{}_v(e)$ is defined analogously. Here is our key definition. We call a graph G to be edge distance- balanced, if $m^{Ga}(e) = m^G{}_b(e)$ holds for each edge $e = ab \in E(G)$.

Definition. Cartesian product: The Cartesian product $G \times H$ of the graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and (a; x)(b; y) is an edge of $G \times H$ if a = b and $xy \in E(H)$, or $ab \in E(G)$ and x = y. Algebraic graph theory can be used to analyze the Cartesian graph product. If the graphG_1 has n_1 vertices and the $n_1 \times n_1$ adjacency matrix A_1, and the graphG_2 has $n_2$vertices and the $n_2 \times n_2$adjacency matrix A_2, then the adjacency matrix of the Cartesian product of both graphs is given by $A_{G1 \times G2} = A_1 \otimes I_{n_2} + A_2 \otimes I_{n_1}$,where $\otimes$ denotes the Kronecker product of matrices and I_n denotes the $n \times n$ identity matrix.

Definition. **cluster G{H}:** The cluster G{H} is obtained by taking one copy of G and |V (G)|copies of a rooted graph H, and by identifying the root of the i^{th} copy of H with the i^{th} vertex of G, i = 1; 2;…,|V (G)|.

Definition. Graph G[H]: The lexicographic product G = G[H] of graphs G and H with disjoint vertex sets V (G) and V (H) and edge sets E(G) and E(H) is the graph with vertex set V (G) × V (H) and u = (u_1; v_1) is adjacent with v = (u_2; v_2) whenever (u_1 is adjacent to u_2) or (u_1 = u_2 and v_1 is adjacent to v_2).

Theorem. Suppose that G and H are Distance balanced graph. Then Co-PI $(G \times H) = 0$

Proof. By theorem2.1 of (tavakoli, 2013), we have, if G and H be edge and vertex distance-balanced graphs. Then G ×H is edge distance-balanced graphs .we knowing that:
$m^{(G \times H)}{}_{(a;x)}(e) = m^{Ga}(ab)|V(H)| + n^{G}{}_{a}(ab)|E(H)|$; $m^{(G \times H)}{}_{(b;y)}(e) = m^{Gb}(ab)|V(H)| + n^{G}{}_{b}(ab)|E(H)|$. Since G is edge and vertex distance-balanced, thus we have:
$n^{G}{}_{a}(ab) = n^{G}{}_{b}(ab)$ and $m^{G}{}_{a}(ab) = m^{G}{}_{b}(ab)$. Therefore, in this case we have $m^{(G \times H)}{}_{(a;x)}(e) = m^{(G \times H)}{}_{(b;y)}(e)$. In a similar way we can see that, for every edge e of B, we have $m^{(G \times H)}{}_{(a;x)}(e) = m^{(G \times H)}{}_{(b;y)}(e)$. Thus by definition of Co-PI index we have:
CO-PI (G×H) = 0. ■

Theorem . CO-PI (G {H}) = |E (G{H}| (E|(H)|(|V(G)|-1)+|E(G)|)+CO-PI(G)

Proof.
CO-PI(G{H}) =
$$\sum_{e=uv \in G\{H\}} (m_u^{G\{H\}} - m_v^{G\{H\}}) = \sum_{e=uv \in G\{H\}} (|E(H)|(|V(G)|-1) + |E(G)|) + \sum_{e=ab \in H} m_a^{(H)} - \sum_{e=ab \in H} m_b^{(H)}$$
= |E(G{H}| (E|(H)|(|V(G)|-1)+|E(G)|)+CO-PI(G), which completed the proof.■■

Theorem. Suppose that f H is triangle-free and regular graph. Then CO-PI(G[H}) = 0.

Proof. We prove that G [H] is edge distance-balanced graph. Since, H is triangle-free and regular graph, for each e = (a; x)(b; y) ∈ E(G[H]), we have $m^{G[H]}{}_{(a;x)}(e) = m^{G[H]}{}_{(b;y)}(e)$ and thus G[H] is edge distance-balanced and CO-PI(G[H}) = 0. ■

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