Estimating the Vertex *PI* Index

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The vertex *PI* index is a distance-based molecular structure descriptor, that recently found numerous chemical applications. Lower and upper bounds for *PI* are obtained, as well as results of Nordhaus-Gaddum type. Also a relation between the Szeged and vertex *PI* indices is established.

Key words: Molecular Graph; Vertex *PI* Index; Edge *PI* index; Molecular Structure Descriptor; Topological Index; Distance (in Graph); Estimating the Vertex *PI* Index

1. Introduction

In theoretical chemistry molecular-graph based structure descriptors – also called topological indices – are used for modelling physico-chemical, pharmacologic, toxicologic, etc. properties of chemical compounds [1, 2]. There exist several types of such indices, reflecting different aspects of the molecular structure. Arguably the best known of these indices is the Wiener index $W = W(G)$, equal to the sum of distances between all pairs of vertices of the molecular graph G [1, 3 – 5]. The Szeged index [6 – 8] is closely related to the Wiener index and coincides with it in the case of trees. In the notation explained below, the Szeged index is defined as

$$Sz = Sz(G) = \sum_{e\in E(G)} n_1(e|G)n_2(e|G). \tag{1}$$

In view of the considerable success of the Szeged index in chemical graph theory (for details see the review [8] and the book [9]), an additive version of it has recently been put forward, called the vertex *PI* index [10, 11]:

$$PI = PI(G) = \sum_{e\in E(G)} [n_1(e|G) + n_2(e|G)]. \tag{2}$$

Earlier, a similar quantity, referred here as the edge *PI* index and denoted by PI_e, was considered [12, 13]:

$$PI_e = PI_e(G) = \sum_{e\in E(G)} [m_1(e|G) + m_2(e|G)]. \tag{3}$$

The notation used in (1) – (3) is explained below.

Numerous applications of PI_e were reported [9, 14, 15]. It was shown that the edge *PI* index correlates well with the Wiener and Szeged indices and these all correlate with a variety of physico-chemical properties and biological activities of a large number of diverse and complex compounds [9, 14, 16]. Recently, several mathematical properties of the two *PI* indices were established [11, 12, 17 – 22]. The present paper is aimed at contributing more results along the same lines.

Let $G = (V,E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. Let $t(G)$ be the number of triangles in G. For $v_i \in V(G)$, the degree (= number of first neighbours) of the vertex v_i is denoted by $\deg(v_i)$. For $v_i, v_j \in V(G)$, the length of the shortest path between the vertices v_i and v_j is their distance $d(v_i, v_j|G)$. Then

$$W = W(G) = \sum_{1\le i<j\le n} d(v_i, v_j|G).$$

The maximum distance in the graph G is its diameter, denoted by d.

Let e be an edge of the graph G, connecting the vertices v_i and v_j. Define two sets $N_1(e|G)$ and $N_2(e|G)$ as

$$N_1(e|G) = \{v_k \in V(G) | d(v_k, v_i|G) < d(v_k, v_j|G)\},$$

$$N_2(e|G) = \{v_k \in V(G) | d(v_k, v_j|G) < d(v_k, v_i|G)\}.$$

The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$, respectively. Thus, $n_1(e|G)$ counts the vertices of G lying closer to the vertex v_i than to the vertex v_j. The meaning of $n_2(e|G)$ is analogous. Vertices equidistant from both ends of the edge v_iv_j belong neither to $N_1(e|G)$ nor to $N_2(e|G)$. Note that for any edge e of G, $n_1(e|G) \geq 1$ and $n_2(e|G) \geq 1$, because $v_i \in N_1(e|G)$ and $v_j \in N_2(e|G)$.

The Szeged and the vertex *PI* indices are then defined via (1) and (2), respectively. In (3), by $m_1(e|G)$ is denoted the number of edges of G lying closer to the vertex v_i than to the vertex v_j; the meaning of $m_2(e|G)$ is analogous.

Recall that for any tree T,

$$W(T) = \sum_{e\in E(T)} n_1(e|T)n_2(e|T) \equiv Sz(T),$$

a result recognized already by Wiener in his seminal paper [23]. Interestingly, the equality $W = Sz$ holds also for the complete graph K_n.

For any n-vertex tree T and for the complete graph K_n it is

$$PI(T) = PI(K_n) = n(n-1). \tag{4}$$

The rest of the paper is structured as follows. In Section 2 we give lower and upper bounds for *PI*. In Section 3 we obtain a Nordhaus-Gaddum type result for *PI*. In Section 4 we discuss the relation between the Szeged and the vertex *PI* indices.

2. Lower and Upper Bounds on Vertex *PI* Index

Theorem 2.1 *Let G be a connected graph on n vertices, m edges, and diameter d. Then*

$$PI(G) \geq 2m + d^2 - d \tag{5}$$

with equality holding if and only if $G \cong K_n$ or $G \cong P_n$ (where by P_n is denoted the n-vertex path [1]).

Proof. For each edge $e \in E(G)$, we have

$$n_2(e|G) + n_1(e|G) \geq 2.$$

Since G has diameter d, the path P_{d+1} is contained in G. Thus we have

$$PI(G) \geq PI(P_{d+1}) + \sum_{e\in E(G)\setminus E(P_{d+1})} [n_1(e|G) + n_2(e|G)] \tag{6}$$

$$\geq d(d+1) + 2(m-d). \tag{7}$$

The vertex *PI* indices of P_n and K_n are given by (4). From these one can easily check that equality in (5) holds for these two graphs.

Suppose now that equality holds in (5). Then equality must hold in (6) and (7). We need to consider two cases: (a) $m = d$, (b) $m > d$.

Case (a): $m = d$. From equality in (6), we must have $n = m+1$ and hence $G \cong P_n$.

Case (b): $m > d$. From equality in (7) follows that for any $e \in E(G) \setminus E(P_{d+1})$,

$$n_1(e|G) = n_2(e|G) = 1. \tag{8}$$

Since G is connected, by equality in (6) and (8), we conclude that there exists a vertex $v_i \in V(G) \setminus V(P_{d+1})$, such that $d(v_i, v_j|G) = 1$ for any $v_j \in V(P_{d+1})$. Therefore the diameter of G is at most 2. Suppose that $P_{d+1} = v_1v_2 \ldots v_{d+1}$. Since $v_iv_1 = e \in E(G) \setminus E(P_{d+1})$, and $v_iv_{d+1} \in E(G)$, by (8) we must have $v_1v_{d+1} \in E(G)$. Thus the diameter of G is 1 and hence $G \cong K_n$. □

Lemma 2.2 *Let G be a simple graph of order n, possessing $t(G)$ triangles. Then*

$$\sum_{v_iv_j\in E(G)} |N_i \cap N_j| = 3t(G),$$

where $|N_i \cap N_j|$ is the number of common neighbours of v_i and v_j.

We now give an upper bound on the vertex *PI* index in terms number of vertices n, number of edges m, and number of triangles $t(G)$ in G.

Theorem 2.3 *Let G be a connected graph with $n > 2$ vertices and m edges. Also let $t(G)$ be the number of triangles of G. Then*

$$PI(G) \leq nm - 3t(G). \tag{9}$$

Moreover, the equality holds in (9) if and only if G is a bipartite graph or $G \cong K_3$.

Proof. We have

$$PI(G) = \sum_{e\in E(G)} [n_1(e|G) + n_2(e|G)] \leq \sum_{e\in E(G)} (n - |N_i \cap N_j|) = nm - 3t(G), \tag{10}$$

which completes the first part of the proof.

Now we have to show that the equality holds in (9) if and only if G is a bipartite graph or $G \cong K_3$. For a bipartite graph G, we have $n_1(e|G)+n_2(e|G)=n$ for any edge $e \in E(G)$ as well as $t(G)=0$ and hence $PI(G)=nm$ holds. For $G \cong K_3$, we have $n_1(e|G)+n_2(e|G)=2$ for any edge $e \in E(G)$ and $t(G)=1$. Hence $PI(G)=6=nm-t(G)$ holds. Thus the equality holds in (9) if G is a bipartite graph or $G \cong K_3$.

Suppose now that the equality holds in (9). Then the equality holds also in (10). From equality in (10) follows that for any edge $e=v_iv_j \in E(G)$,

$$n_1(e|G)+n_2(e|G)=n-|N_i \cap N_j|. \tag{11}$$

By contradiction, we show that G is a bipartite graph or $G \cong K_3$. For this we suppose that G is neither bipartite nor $G \cong K_3$. If so, then G contains an odd-membered cycle C_{2p+1} and has at least 4 vertices. Since G is connected, there exists an edge $e=v_iv_j \in E(C_{2p+1})$, such that $n_1(e|G)+n_2(e|G)<n-|N_i \cap N_j|$, a contradiction, by (11). □

3. Nordhaus-Gaddum Type Results for the Vertex *PI* Index

For a graph G, the chromatic number $\chi(G)$ is the minimum number of colors needed to color the vertices of G in such a way that no two adjacent vertices are assigned the same color. In 1956, Nordhaus and Gaddum [24] gave bounds involving the chromatic number $\chi(G)$ of a graph G and its complement $\overline{G}$:

$$2\sqrt{n} \le \chi(G)+\chi(\overline{G}) \le n+1.$$

Motivated by the above results, we now obtain analogous conclusions for the vertex *PI* index.

We first observe that for $n \ge 5$,

$$\begin{aligned}2PI(\overline{P}_n) &= 2(3+4+\underbrace{5+5+\cdots+5}_{n-4}) \\ &\quad +2(4+5+\underbrace{6+6+\cdots+6}_{n-5}) \\ &\quad +2(3+4+5+\underbrace{6+6+\cdots+6}_{n-6}) \\ &\quad +(n-6)(4+4+5+5+\underbrace{6+6+\cdots+6}_{n-7}) \\ &= 2(5n-13)+2(6n-21) \\ &\quad +2(6n-24)+(6n-24)(n-6)\end{aligned}$$

that is,

$$PI(\overline{P}_n)=(n-2)(3n-7).$$

Theorem 3.1 *Let G be a connected graph on $n \ge 5$ vertices, diameter d, and with a connected complement $\overline{G}$. Then*

$$PI(G)+PI(\overline{G}) \ge n(n-1)+(d-1)(3d-4) \tag{12}$$

with equality holding if and only if $G \cong P_n$.

Proof. Since G has diameter d, then $\overline{P}_{d+1}$ is a subgraph of $\overline{G}$. Thus

$$\begin{aligned}PI(\overline{G}) &\ge PI(\overline{P}_{d+1}) \\ &\quad + \sum_{e \in E(\overline{G}) \setminus E(\overline{P}_{d+1})} [n_1(e|\overline{G})+n_2(e|\overline{G})] && (13) \\ &\ge (d-1)(3d-4)+2\left[\overline{m}-\frac{1}{2}d(d-1)\right] && (14) \\ &= 2(d-1)(d-2)+n(n-1)-2m. && (15)\end{aligned}$$

From (5) and (15) we get

$$PI(G)+PI(\overline{G}) \ge 2(d-1)(d-2)+n(n-1)+d^2-d \tag{16}$$

and inequality (12) follows.

Suppose now that equality holds in (12). Then equality holds in (13), (14), and (16). Using the same way of reasoning as in the proof of Theorem 2.1, we conclude that $G \cong P_n$.

Conversely, one can easily check that (12) holds for $G \cong P_n$. □

It was first observed by Goodman [25] that $t(G)+t(\overline{G})$ is determined by the vertex degree sequence:

Lemma 3.2 [25] *Let $t(G)$ and $t(\overline{G})$ be, respectively, the number of triangles in G and $\overline{G}$. Then*

$$\begin{aligned}t(G)+t(\overline{G}) &= \frac{1}{2}\sum_{i=1}^{n} \deg(v_i)^2-(n-1)m \\ &\quad + \frac{1}{6}n(n-1)(n-2).\end{aligned}$$

A molecular structure-descriptor introduced long time ago [2,26] is the so-called first Zagreb index (M_1) equal to the sum of squares of the degrees of all vertices. Some basic properties of M_1 can be found in [27,28]. Now we are ready to give upper bound for $PI(G)+PI(\overline{G})$:

Theorem 3.3 *Let G be a connected graph on $n > 2$ vertices, m edges, diameter d, $t(G)$ triangles, and with a connected complement $\overline{G}$. Then*

$$PI(G) + PI(\overline{G}) \leq (n-1)(3m+n) - \frac{3}{2}M_1(G). \quad (17)$$

Moreover, the equality holds in (17) if and only if $G \cong P_4$.

Proof. Let $\overline{m}$ be the number of edges of $\overline{G}$. By (9), we get

$$PI(G) + PI(\overline{G}) \leq n(m+\overline{m}) - 3[t(G) + t(\overline{G})] \quad (18)$$

$$= \frac{1}{2}n^2(n-1) - \frac{3}{2}\sum_{i=1}^{n}\deg(v_i)^2 + 3(n-1)m - \frac{1}{2}n(n-1)(n-2). \quad (19)$$

Since $m + \overline{m} = n(n-1)/2$, inequality (17) is obtained from (19).

Suppose now that equality holds in (17). Then equality holds in (18). From (9) we conclude that both G and $\overline{G}$ are bipartite graphs. So we may assume that $V(G) = A \cup B$ and $A \cap B = \emptyset$. Since $\overline{G}$ is also bipartite, we must have $|A| \leq 2$ and $|B| \leq 2$. Further, since both G and $\overline{G}$ are connected, it must be $G \cong P_4$.

Conversely, one can easily check that (17) holds for $G \cong P_4$. □

4. Relation Between Szeged Index and Vertex *PI* Index

In this section we obtain a relation between Szeged and vertex *PI* indices. For this we need the following:

Lemma 4.1 [29] *Let $(a_1, a_2, \ldots, a_p)$ and $(b_1, b_2, \ldots, b_p)$ be two positive n-tuples such that there exist positive numbers x_1, X_1, x_2, X_2 satisfying:*

$$0 < x_1 \leq a_i \leq X_1 \ \text{ and } \ 0 < x_2 \leq b_i \leq X_2 \quad \text{for } \ i = 1, 2, \ldots, p.$$

Then

$$\sum_{i=1}^{p} a_i^2 \sum_{i=1}^{p} b_i^2 - \left(\sum_{i=1}^{p} a_i b_i\right)^2 \leq \frac{1}{4}p^2(X_1X_2 - x_1x_2)^2.$$

Theorem 4.2 *Let G be a simple graph with n vertices and m edges. Also let Sz and PI be the Szeged and vertex PI indices, respectively, of G. Then*

$$16mSz - 4PI^2 \leq m^2(n-3)^2. \quad (20)$$

Equality in (20) holds if and only if $G \cong \overline{K}_n$ or $G \cong K_3$ or $G \cong \overline{P}_3$.

Proof. For each edge $e \in E(G)$,

$$\frac{n_1(e|G) + n_2(e|G)}{2} \geq \sqrt{n_1(e|G)n_2(e|G)} \quad (21)$$

from which follows

$$\sum_{e\in E(G)} (n_1(e|G) + n_2(e|G))^2 \geq 4 \sum_{e\in E(G)} n_1(e|G)n_2(e|G). \quad (22)$$

Setting into Lemma 4.1 $p = m$, $a_i = n_1(e_i|G) + n_2(e_i|G)$, $i = 1, 2, \ldots, m$, $x_1 = \min_i a_i$, $X_1 = \max_i a_i$, and $b_1 = b_2 = \cdots = b_m = 1$, $x_2 = X_2 = 1$, we get

$$m \sum_{e\in E(G)} [n_1(e|G) + n_2(G)]^2 \leq \left[\sum_{e\in E(G)} (n_1(e|G) + n_2(G))\right]^2 + \frac{1}{4}m^2(X_1 - x_1)^2. \quad (23)$$

We have $X_1 \leq n$ and $x_1 \geq 2$. If $X_1 \leq n-1$, then $X_1 - x_1 \leq n-3$. Otherwise, $X_1 = n$. In that case we must have $x_1 \geq 3$. Thus for both cases $X_1 - x_1 \leq n-3$. Using this as well as (22) and (23), we get the required result (20).

Suppose that the equality holds in (20). Then all inequalities in the above argument must be equalities. Thus from equality in (21) and (22), we get that for each edge $e \in E(G)$,

$$n_1(e|G) = n_2(e|G).$$

From equality in (23) and using above result, we get

$$m^2(n-3)^2 = 0.$$

Thus either $m = 0$ or $n = 3$, that is, either $G \cong \overline{K}_n$ or $G \cong K_3$ or $G \cong \overline{P}_3$.

Conversely, one can easily verify that (20) holds for $G \cong \overline{K}_n$, $G \cong K_3$, and $G \cong \overline{P}_3$. □

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