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Bound for Vertex PI Index in Terms of Simple Graph Parameters

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Abstract. The vertex *PI* index is a distance–based molecular structure descriptor, that recently found numerous chemical applications. In this letter we obtain a lower bound on the vertex *PI* index of a connected graph in terms of number of vertices, edges, pendent vertices, and clique number, and characterize the extremal graphs.

1. Introduction

In theoretical chemistry molecular–graph based structure descriptors – also called topological indices – are used for modeling physico–chemical, pharmacologic, toxicologic, etc. properties of chemical compounds ([4, 12]). There exist several types of such indices, reflecting different aspects of 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 ([4, 12]). The Szeged index is closely related to the Wiener index and coincides with it in the case of trees [3, 5, 10, 12]. In the notation explained below, it is defined as

$$Sz = Sz(G) = \sum_{e=v_iv_j\in E(G)} n_i(e|G)\, n_j(e|G)\ . \tag{1}$$

In view of the considerable success of the Szeged index (for details see the review [5] and the book [3]), an additive version of it has been put forward, called the vertex *PI* index [9]:

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

Its basic mathematical properties were established in a number of recent papers [2, 6, 9, 11, 13]. At this point it is worth noting that in chemical graph theory also an edge *PI* index has been considered [3, 8].

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Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. For $v_i \in V(G)$, the degree (= number of first neighbors) of the vertex v_i is denoted by d_i.

For $v_r, v_s \in V(G)$, the length of the shortest path between the vertices v_r and v_s is their distance, $d(v_r, v_s|G)$.

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

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

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

The number of elements of $N_i(e|G)$ and $N_j(e|G)$ are denoted by $n_i(e|G)$ and $n_j(e|G)$, respectively. Thus, $n_i(e|G)$ counts the vertices of G lying closer to the vertex v_i than to the vertex v_j. The meaning of $n_j(e|G)$ is analogous. Vertices equidistant from both ends of the edge v_iv_j belong neither to $N_i(e|G)$ nor to $N_j(e|G)$. Note that for any edge $e = v_iv_j$ of G, $n_i(e|G) \geq 1$ and $n_j(e|G) \geq 1$, because $v_i \in N_i(e|G)$ and $v_j \in N_j(e|G)$. The Szeged and the vertex PI indices are then defined via Eqs. (1) and (2).

For any n-vertex tree T as well as for the complete graph K_n,

$$PI(T) = PI(K_n) = n(n-1).$$

Denote by $H(n, \omega)$, $\omega \leq n-1$, is the graph on n vertices consisting of a clique on ω vertices and randomly connect $n-\omega$ pendent to arbitrary vertices of K_ω. It is easily verified that $PI(H(n, \omega)) = n(n-1)$.

In this paper we obtain a lower bound on the vertex PI index of a connected graph G in terms of the number of vertices (n), edges (m), pendent vertices (p), and clique number (ω), and characterize the extremal graphs.

2. Lower bounds on vertex PI index

For bipartite graph G ($\omega = 2$), $PI(G) = mn$. So it is interesting to find the lower bound on PI index for $\omega \geq 3$:

Theorem 2.1. *Let G be a connected graph with n vertices, m edges, p pendent vertices, and clique number ω ($\omega \geq 3$). Then*

$$PI(G) \geq 2m + (n-2)p + (n-\omega)(\omega-1) \tag{3}$$

with equality holding if and only if $G \cong K_n$ or $G \cong H(n, \omega)$.

Proof. If G is isomorphic to the complete graph K_n, then $m = n(n-1)/2$, $\omega = n$, $p = 0$ and hence the equality holds in (3). Therefore we may assume that $G \not\cong K_n$, in which case $\omega \leq n-1$.

For each edge $e = v_iv_j \in E(G)$,

$$n_i(e|G) + n_j(e|G) \geq 2. \tag{4}$$

If e is a pendent edge, then

$$n_i(e|G) + n_j(e|G) = n. \tag{5}$$

Since G has clique number ω ($\omega \geq 3$), the complete graph K_ω is contained in G. Suppose that $V(K_\omega) = \{v_1, v_2, \ldots, v_\omega\}$, $\omega \geq 3$ and $\mathbf{S} = V(G) \setminus V(K_\omega) = \{v_{\omega+1}, v_{\omega+2}, \ldots, v_n\}$. Then $|\mathbf{S}| = n - \omega > 0$.

Case(i) : We first assume that there exist two vertices v_s, $v_t \in V(K_\omega)$ such that $d(v_i, v_s|G) \neq d(v_i, v_t|G)$ for all $v_i \in \mathbf{S}$. Let $d(i) = \min\{d(v_i, v_j|G) \mid v_j \in V(K_\omega)\}$. Suppose that $d(i)$ is the smallest distance between the vertex v_i and any vertex in $\mathbf{R} = \{v_1, v_2, \ldots, v_r\} \subseteq V(K_\omega)$. Then $d(v_i, v_j|G) > d(i)$ for any vertex v_j in $V(K_\omega) \setminus \mathbf{R} = \{v_{r+1}, v_{r+2}, \ldots, v_\omega\} = \mathbf{R}'$. For any edge $e = v_jv_k \in E(K_\omega)$, $v_j \in \mathbf{R}$, $v_k \in \mathbf{R}'$. Denote by $N_{jk}(e|G)$ the union $N_j(e|G) \cup N_k(e|G)$.

Then the vertex $v_i \in \mathbf{S}$ belongs to $r(\omega - r)$ sets $N_{jk}(e|G)$, $v_j \in \mathbf{R}$, $v_k \in \mathbf{R}'$, that is, the vertex v_i in $\mathbf{S}$ belong to at least $\omega - 1$ sets $N_{jk}(e|G)$, $v_j \in \mathbf{R}$, $v_k \in \mathbf{R}'$. Since K_ω has $\omega(\omega-1)/2$ edges and $n-\omega$ is the number of vertices in $G \setminus K_\omega$ ($|\mathbf{S}| = n - \omega$), we have

$$\sum_{v_jv_k=e\in E(K_\omega)} (n_j(e|G) + n_k(e|G)) \tag{6}$$

$$= \sum_{v_jv_k=e\in E(K_\omega)} \Big(|N_j(e|G)| + |N_k(e|G)| + |N_j(e|G) \cap N_k(e|G)|\Big)$$

as $|N_j(e|G)| = n_j(e|G)$, $|N_k(e|G)| = n_k(e|G)$ and $|N_j(e|G) \cap N_k(e|G)| = 0$

$$= \sum_{v_jv_k=e\in E(K_\omega)} |N_j(e|G) \cup N_k(e|G)| = \sum_{v_jv_k=e\in E(K_\omega)} |N_{jk}(e|G)|$$

$$\geq \omega(\omega-1) + (n-\omega)(\omega-1)\,. \tag{7}$$

Claim 1.

$$\sum_{\substack{v_iv_j=e\in E(G\setminus K_\omega)\\ d_i,d_j>1}} [n_i(e|G) + n_j(e|G)] \geq 2\Big(m - \frac{1}{2}\,\omega(\omega-1) - p\Big) \tag{8}$$

with equality holding if and only if $m = \omega(\omega-1)/2 + p$.

Proof of Claim 1. Since G is connected and $n > \omega$, the number of non-pendent edges in $G \setminus K_\omega$ is equal to $m - \omega(\omega-1)/2 - p$, that is, $m \geq \omega(\omega-1)/2 + p$. By (4), we get the result (8). If $m > \omega(\omega-1)/2 + p$, then at least one non-pendent edge belongs to $G \setminus K_\omega$. Thus there is a non-pendent edge $e = v_jv_k$ such that $v_j \in V(K_\omega)$ and $v_k \in V(G \setminus K_\omega)$, and v_k is not adjacent to all vertices in the set $\{v_1, v_2, \ldots, v_\omega\}$. Thus, $n_j(e|G) + n_k(e|G) \geq 3$ and hence

$$\sum_{\substack{v_iv_j=e\in E(G\setminus K_\omega)\\ d_i,d_j>1}} [n_i(e|G) + n_j(e|G)] > 2\Big(m - \frac{1}{2}\,\omega(\omega-1) - p\Big)\,.$$

This implies that equality in (8) holds if and only if $m = \omega(\omega-1)/2 + p$.

Now,

$$PI(G) = \sum_{v_iv_j=e\in E(G)} [n_i(e|G) + n_j(e|G)]$$

$$= \sum_{\substack{v_iv_j=e\in E(G)\\ d_i \text{ or } d_j=1}} [n_i(e|G) + n_j(e|G)] + \sum_{\substack{v_iv_j=e\in E(G)\\ d_i,d_j>1}} [n_i(e|G) + n_j(e|G)]$$

$$= np + \sum_{v_iv_j=e\in E(K_\omega)} [n_i(e|G) + n_j(e|G)] + \sum_{\substack{v_iv_j=e\in E(G\setminus K_\omega)\\ d_i,d_j>1}} [n_i(e|G) + n_j(e|G)]$$

by (5)

$$\geq np + \omega(\omega-1) + (n-\omega)(\omega-1) + 2\Big(m - \frac{1}{2}\,\omega(\omega-1) - p\Big) \tag{9}$$

by (7) and (8).

From above we get the required result (3).

Case(ii) : We consider the subset $\mathbf{S}'$ of the, set $\mathbf{S}$ $(|\mathbf{S}'| = h > 0)$, whose elements v_i have the property $d(v_i, v_j|G) = d(v_i, v_k|G) = d$ for any two vertices $v_j, v_k \in V(K_\omega)$. Further, let the shortest paths from the vertex v_i to the clique K_ω be

$$v_i\, v_{i_0^{(1)}} v_{i_1^{(1)}} \ldots v_{i_{d-2}^{(1)}}\, v_1, v_i\, v_{i_0^{(2)}} v_{i_1^{(2)}} \ldots v_{i_{d-2}^{(2)}}\, v_2, \ldots, v_i\, v_{i_0^{(\omega)}} v_{i_1^{(\omega)}} \ldots v_{i_{d-2}^{(\omega)}}\, v_\omega\ .$$

It may be that the $v_{i_j^{(r)}}$ and $v_{i_j^{(s)}}$ are the same, $r \neq s$.

Thus we have $v_j \in N_{i\, i_0^{(j)}}(e|G) = N_i(e|G) \cup N_{i_0^{(j)}}(e|G)$, $j = 1, 2, \ldots, \omega$, and hence

$$\sum_{\substack{v_i v_j = e \in E(G\setminus K_\omega) \\ d_i, d_j > 1}} [n_i(e|G) + n_j(e|G)] > h(\omega - 1) + 2\Big(m - \frac{1}{2}\,\omega(\omega - 1) - p\Big)$$

as $|\mathbf{S}'| = h$.

There exist two vertices v_j and $v_k \in V(K_\omega)$ such that $d(v_i, v_j|G) \neq d(v_i, v_k|G)$ for any vertex v_i in $\mathbf{S} \setminus \mathbf{S}'$ $(|\mathbf{S}| - |\mathbf{S}'| = n - h - \omega)$. In addition, since K_ω has $\omega(\omega - 1)/2$ edges, similarly as in **Case (i)**, we have

$$\sum_{v_i v_j = e \in E(K_\omega)} [n_i(e|G) + n_j(e|G)] \geq \omega(\omega - 1) + (n - h - \omega)(\omega - 1)\ .$$

Using the above results, we get

$$\begin{aligned}
PI(G) &= \sum_{v_i v_j = e \in E(G)} (n_i(e|G) + n_j(e|G)) \\
&= \sum_{\substack{v_i v_j = e \in E(G) \\ d_i \text{ or } d_j = 1}} [n_i(e|G) + n_j(e|G)] + \sum_{\substack{v_i v_j = e \in E(G) \\ d_i, d_j > 1}} [n_i(e|G) + n_j(e|G)] \\
&= np + \sum_{e \in E(K_\omega)} (n_i(e|G) + n_j(e|G)) + \sum_{\substack{e \in E(G\setminus K_\omega) \\ d_i, d_j > 1}} [n_i(e|G) + n_j(e|G)] \quad \text{by (5)} \\
&> np + \omega(\omega - 1) + (n - h - \omega)(\omega - 1) + h(\omega - 1) \\
&\qquad + 2\Big(m - \frac{1}{2}\,\omega(\omega - 1) - p\Big)\,. \qquad (10)
\end{aligned}$$

From above we get the required result (3). Hence the first part of the proof is done.

By direct checking one can easily verify that equality in (3) holds for the complete graph K_n and the graph $H(n,\ \omega)$.

Suppose now that equality holds in (3). Then we must have equality also in (9). Then there exist two vertices $v_s,\ v_t \in V(K_\omega)$ such that $d(v_i,\ v_s|G) \neq d(v_i,\ v_t|G)$ for any vertex v_i in $V(G \setminus K_\omega)$. The equality holds also in (7) and (8). From equality in (8), $m = \omega(\omega - 1)/2 + p$. Thus all edges in $G \setminus K_\omega$ pendent and the number of pendent vertices in G is $n - \omega$. Hence $G \cong H(n,\ \omega)$. □

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