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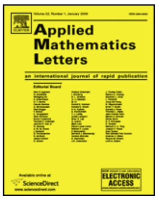

Extremal graphs with respect to the vertex PI index

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ABSTRACT

The vertex PI index of a graph G is the sum over all edges $uv \in E(G)$ of the number of vertices which are not equidistant to u and v. In this paper, the extremal values of this new topological index are computed. In particular, we prove that for each n-vertex graph G, $n(n-1) \leq PI_v(G) \leq n \cdot \lfloor \frac{n}{2} \rfloor \cdot \lceil \frac{n}{2} \rceil$, where $\lfloor x \rfloor$ denotes the greatest integer not exceeding x and $\lceil x \rceil$ is the smallest integer not less than x. The extremal graphs with respect to the vertex PI index are also determined.

1. Introduction

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is denoted by $d(u, v)$ and it is defined as the number of edges in a minimal path connecting them. Define $N_G(u)$ to be the set of all vertices adjacent to u. The diameter $diam(G)$ is the greatest distance between two vertices of G.

Suppose *Graph* denotes the class of all graphs. A map *Top* from *Graphs* into real numbers is called a topological index, if $G \cong H$ implies that $Top(G) = Top(H)$. Obviously, the maps Top_1 and Top_2 defined as the number of edges and vertices, respectively, are topological indices.

The Wiener index was the first reported topological index based on graph distances, see [1]. This index is defined as the sum of all distances between vertices of the graph under consideration. We encourage the reader to consult the special issues of MATCH Communication in Mathematics and in Computer Chemistry [2], Discrete Applied Mathematics [3] and [4,5], for more information on the Wiener index, the chemical applications of the index and its history.

Let $e = uv$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that vertices equidistant to u and v are not counted. The vertex PI index of G is defined as $PI_v(G) = \sum_{e=uv}[n_u(e) + n_v(e)]$, [6]. This index is a vertex variant of another topological index named PI index, see for details [7–11].

For the sake of completeness we state here a result of [6] which is crucial throughout the paper.

Lemma 1. *Let G be an n-vertex graph, $n \geq 4$. Then $PI_v(G) \leq |E(G)||V(G)|$ with equality if and only if G is bipartite.*

Throughout this paper, we only consider connected graphs. The floor of a real number x, written $\lfloor x \rfloor$, is the greatest integer not exceeding x and the ceiling of x, written $\lceil x \rceil$, is the smallest integer not less than x. Our notation is standard and is taken mainly from [12–14].

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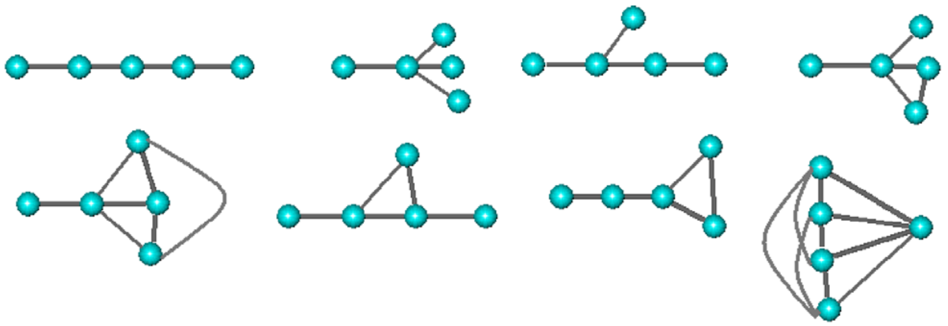

Fig. 1. The elements of X_5.

2. Main results

In this section we present a new formula for computing the vertex PI index of a graph. Then we apply this formula to obtain the extremal graphs with respect to the vertex PI index.

Lemma 2. *Let G be a connected graph. Then* $PI_v(G) = \sum_{x \in V(G)} m_x(G)$, *where* $m_x(G) = |\{e = uv \in E(G) \mid d(x, u) \neq d(x, v)\}|$.

Proof. We apply double counting to the set of ordered pairs (x, e) for which $x \in V(G)$, $e = uv \in E(G)$ and $d(x, u) \neq d(x, v)$. Choose $x \in V(G)$ and $f = ab \in E(G)$. Define $n_f(G) = |\{v \in V(G) \mid d(a, v) \neq d(b, v)\}|$. One can see that, on the one hand, the number of pairs is $\sum_{f \in E(G)} n_f(G) = PI_v(G)$. On the other hand, $\sum_{x \in V(G)} m_x(G) = \sum_{f \in E(G)} n_f(G)$. Therefore, $PI_v(G) = \sum_{x \in V(G)} m_x(G)$, as desired. □

Theorem 1. *Let G be n-vertex graph,* $n \geq 4$. *Then* $PI_v(G) \leq n\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ *with equality if and only if G is a complete bipartite graph with balanced bipartition.*

Proof. Suppose $\mathcal{G}_n$ is the set of all n-vertex graphs. We will prove:

$$PI_v(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) = \text{Max}\{PI_v(H) \mid H \in \mathcal{G}_n\}.$$

Suppose $H \in \mathcal{G}_n$ and fix a vertex $x \in V(H)$. Define $d = \text{Max}\{d(x, y) \mid y \in V(H)\}$ and $A_i = \{y \in V(H) \mid d(x, y) = i\}$, $0 \leq i \leq d$. Consider x as a root of H and draw H in such a way that the elements of A_i constitute the distance level i with respect to x. Then one can see that H has exactly two types of edges, the edges between vertices of A_i, $0 \leq i \leq d$, and the edges connecting vertices of A_j and those of A_{j+1}, $0 \leq j \leq d - 1$. By Lemma 2, $PI_v(H) = \sum_{x \in V(H)} m_x(H)$. To maximize PI_v, we must maximize the values of $m_x(H)$, $x \in V(H)$. If $a_i = |A_i|$, $0 \leq i \leq d$, then the number of second type edges of H is at most $s = a_0a_1 + a_1a_2 + a_2a_3 + \cdots + a_{d-1}a_d$. Since this number is equal to $m_x(H)$ and $n = a_0 + a_1 + \cdots + a_d$, s attains its maximum if and only if $d = 2$ and $a_1 - a_2 \leq 1$. On the other hand, $PI_v(G)$ attains its maximum if and only if $m_x(G)$ is maximum, for every vertex $x \in G$. Therefore, H is a complete bipartite graph with $m = \lceil \frac{n-1}{2} \rceil + \lceil \frac{n-1}{2} \rceil \times \lfloor \frac{n-1}{2} \rfloor = \lceil \frac{n}{2} \rceil \times \lfloor \frac{n}{2} \rfloor$. Apply Lemma 1, we have $PI_v(H) \leq mn = \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$. Our proof shows that the equality is satisfied if and only if the graph is complete bipartite with balanced bipartition. □

Below we use the terminology and notation given in the proof of Theorem 1. Suppose X_n is the set of all n-vertex graphs G with the property that if G has an even cycle $v_1, \ldots, v_{k-1}, v_1$ then there are unique integers s, t, $1 < s < t < k - 1$, such that $v_s, \ldots, v_t$ are vertices of a layer which constitutes a clique, $v_i \in A_{i-1}$, $1 \leq i \leq s$, and $v_{t+j} \in A_{s-j}$, $1 \leq j \leq s$.

Example 1. Suppose P_n, S_n and K_n denote the path, star and complete graphs with exactly n vertices. Then $X_3 = \{P_3, K_3\}$ and $X_4 = \{P_4, S_4, K_4\}$. The elements of X_5 are depicted in Fig. 1.

Theorem 2. *Let G be n-vertex graph. Then* $PI_v(G) \geq n(n - 1)$ *with equality if and only if* $G \in X_n$.

Proof. Suppose G_u denotes the rooted graph of G at u, for a vertex $u \in V(G)$. Define $d = \text{Max}\{d(u, y) \mid y \in V(G)\}$ and $A_i = \{y \in V(G) \mid d(u, y) = i\}$, $0 \leq i \leq d$. Then $m_u(G) \geq \sum_{i=1}^{d} |A_i| = n - 1$ and so $PI_v(G) \geq n(n - 1)$. In a similar way as in the proof of Theorem 1, one can see that G_u has exactly two types of edges, the edges connecting vertices of A_i, $0 \leq i \leq d$, and the edges between vertices of A_j and those of A_{j+1}, $0 \leq j \leq d - 1$. We now assume that $PI_v(G) = n(n - 1)$. Then $m_u(G) = n - 1$, for each vertex $u \in V(G)$. This implies that the graph H obtained from G by deleting edges of the first type is a spanning tree of G_u containing the root u. So, G_u does not have an even length cycle with all edges of second type.

Suppose G_u has a cycle of even length containing edges of both of the first and second types and also assume that the first type edges is taken from distinct layers of G_u. Between all such cycles, we choose an even cycle C containing shortest paths of G_u. Then by choosing a vertex v from edges of the first type, the rooted graph G_v has a cycle of even length with all edges of second type, a contradiction. Finally, we assume that G_u has a cycle of even length containing the root u, two vertices in the first layer, two vertices in the second layer, …, two vertices in the $(r - 1)$th layer and t vertices $v_1, \ldots, v_t$ in the rth layer of G_u. Choose two non-adjacent vertices v_i and v_j, $i < j$, such that v_j is the first non-adjacent vertex of v_i. Consider the rooted graph G_{v_i}. Since $d(v_i, u) = d(v_j, u)$ and $d(v_i, v_j) = 2$, we obtain a new cycle $C' : v_i, v_{j-1}, v_j, P_1, P_2$, where P_1 is a shortest path connecting v_j and u, and P_2 is a shortest path connecting u and v_i. But P_1 and P_2 have the same length and so C' is a cycle of even length in G_{v_i}, which is impossible. Therefore, the t vertices of the rth layer of G_u induced a clique in G_u. This proves that $G \in X_n$. To complete the proof, we must show that the vertex PI index of the elements of X_n is equal to $n(n-1)$. By definition, $m_u(G)$ is the number of second type edges of G_u. So, the graph L obtained from G_u by deleting the edges of first type is a tree. This shows that $m_u(G) = n - 1$, which completes the proof. □

Open Question: What is the second minimal and maximal graphs with respect to the vertex PI index?

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