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A NOTE ON THE VERTEX PI INDEX OF GRAPHS

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Abstract. Let us consider G be a graph and $e = uv$ an edge of G. Denote by $n_u(e)$ the number of vertices lying closer to the vertex u than the vertex v, and define $n_v(e)$ by analogy. By definition, the vertex PI index of G is given by $PI_v(G) = \sum_{e=uv\in E(G)} [n_u(e) + n_v(e)]$. Suppose G is a triangle free graph. In this paper, it is proved that $PI_v(G) \geq M_1(G)$ with equality if and only if $\mathrm{diam}(G) = 2$, where $M_1(G) = \sum_{v\in V(G)} \deg_G(v)^2$ is the first Zagreb index and $\mathrm{diam}(G)$ denotes the diameter of the graph G. Moreover, we show that the condition of "triangle free" cannot be omitted.

1. INTRODUCTION

A function Top from the class of graphs into real numbers with the property that $\mathrm{Top}(G) = \mathrm{Top}(H)$ whenever G and H are isomorphic is known as a *topological index* in the chemical literature, see [5]. There are many examples of such functions, especially those based on distances, which are applicable in chemistry. The *Wiener index*, defined as the sum of all distances between pairs of vertices in a graph, is probably the first and most studied such graph invariant, both from a theoretical and practical point of view, [3], [11].

The *vertex-PI index* of a graph G was introduced by one of us very recently. It is defined as $PI_v(G) = \sum_{e=uv\in E(G)} [n_u(e) + n_v(e)]$, where $n_u(e)$ denotes the number of vertices lying closer to the vertex u than the vertex v, and $n_v(e)$ is defined analogously, see [1, 7, 8, 9] for details.

Throughout the paper, we only consider simple connected graphs. For a graph G, $V(G)$ and $E(G)$ denote the vertex and edge set, respectively. Given a graph G, the length of a minimal path connecting vertices x and y of G is called the *distance* between them. The diameter $\mathrm{diam}(G)$ of the graph G is defined as the maximum value of distances between vertices of G. We denote this number by $d_G(x, y)$ or $d(x, y)$ for short, [4]. Our notation is standard and taken mainly from the standard book of graph theory.

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2. MAIN RESULTS

In [6], Khadikar proposed a molecular structure descriptor, that in what follows we call the edge-PI index. The edge-PI index is defined as

$$PI(G) = \sum_{e=uv \in E(G)} [m_u(e) + m_v(e)],$$

where the quantities $m_u(e)$ and $m_v(e)$ are the edge-variants of the numbers $n_u(e)$ and $n_v(e)$. More precisely: if $f = st$ is an edge and x a vertex of the connected graph G, then the distance between f and x is equal to $\min\{d(s,x), d(t,x)\}$. Then for $e = uv$ being an edge of the graph G, $m_u(e)$ is the number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v. Analogously, $m_v(e)$ is the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that edges equidistant to u and v are not counted. The vertex PI index of graphs is a vertex variant of the edge PI index.

Deng [2], showed that $PI_e(G) \geq M_1(G) - 2|E(G)|$ with equality if and only if G is a complete multipartite graph, where $M_1(G) = \sum_{v \in V(G)} \deg_G(v)^2$. The aim of this note is to investigate the similar inequality for the vertex-PI index of graphs. We prove that:

Theorem 2.1. *Let G be a triangle free graph. Then $PI_v(G) \geq M_1(G)$ with equality if and only if* $\mathrm{diam}(G) = 2$.

Proof. Suppose $e = uv \in E(G)$ is arbitrary. Since G is triangle free, adjacent vertices of v other u are closer to v than u. This implies that

$$n_u(e) + n_v(e) \geq \deg_G(u) + \deg_G(v).$$

Thus,

$$\begin{aligned} PI_v(G) &= \sum_{e=uv \in E(G)} [n_u(e) + n_v(e)] \\ &\geq \sum_{e=uv \in E(G)} [\deg_G(u) + \deg_G(v)] \\ &= \sum_{v \in V(G)} \deg_G(v)^2 = M_1(G). \end{aligned}$$

We now assume that $\mathrm{diam}(G) = 2$ and there exists an edge $e = uv$ such that $n_u(e) + n_v(e) > \deg_G(u) + \deg_G(v)$. Then there exists a vertex x such that $d_G(u,x) \neq 1$ and $d_G(x,v) \neq 1$. Suppose x is closer to u than v. Hence $d_G(x,v) > d_G(x,u) \geq 2$, which contradicts by our assumption that $\mathrm{diam}(G) = 2$. Therefore, for each edge $e = uv$, $n_u(e) + n_v(e) = \deg_G(u) + \deg_G(v)$ and so $PI_v(G) = M_1(G)$. Conversely, we assume that $PI_v(G) = M_1(G)$. So, for each edge $e = uv$, $n_u(e) + n_v(e) = \deg_G(u) + \deg_G(v)$. If $\mathrm{diam}(G) > 2$ then there exists a path $P : x, y, z, t$ of length 3. Suppose $e = xy$. Since $d_G(t, y) = 2$, t is adjacent to x, which is impossible. □

The condition of "triangle free" in previous theorem cannot be omitted. To do this, we find two graphs G and H such that $PI_v(G) < M_1(G)$ and $PI_v(H) > M_1(H)$. Suppose G is the complete graph K_3. Then a simple calculation shows that $PI_v(G) = 6$ and $M_1(G) = 12$. So, $PI_v(G) < M_1(G)$. Next assume that H is the bridge graph $B(G_1, G_2)$ [10], where G_1 and G_2 are cycle graphs of lengths 3 and 4, respectively. Then $PI_v(H) = 49$ and $M_1(H) = 38$ and so $PI_v(H) > M_1(H)$.

Suppose G is graph and t is a number such that every edge of G lie in exactly t triangles of G. Then a similar argument as previous theorem shows that

$$n_u(e) + n_v(e) \geq \deg_G(u) + \deg_G(v) - t$$

and so,

$$\begin{aligned} PI_v(G) &= \sum_{e=uv\in E(G)} [n_u(e) + n_v(e)] \\ &\geq \sum_{e=uv\in E(G)} [\deg_G(u) + \deg_G(v) - t] \\ &= \sum_{v\in V(G)} \deg_G(v)^2 - tm = M_1(G) - tm. \end{aligned}$$

with equality if and only if $\mathrm{diam}(G) = 2$.

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