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Order of Magnitude of the PI Index

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Abstract

Deng in [H. Deng, On the PI Index of a Graph, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 649−657] determined the extremal graphs with respect to the PI index among all complete multipartite graphs. He wrote: "we do not know whether K_n is the graph with the maximal PI index among all the simple connected graphs on n vertices". In this paper, we study the problem of the order of magnitude for the PI index. As a consequence, a sequence $\{F_n\}_{n\geq 1}$ of graphs is presented for which $PI(F_n) > PI(K_n)$, for $n > 32$.

1. Introduction

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph. The PI index is a new topological index introduced very recently by Khadikar [9-11]. Let G be a graph. The PI index of G is defined as $PI(G) = \sum_{e=uv\in E(G)}[m_u(v) + m_v(u)]$, where $m_u(v)$ is the number of edges lying closer to u than to v and $m_v(u)$ is defined analogously. The mathematical properties of this new index can be found in recent papers, [1−8,12−14,16−20].

In [7], Deng proved that $PI(G) \geq M_1(G) - 2m$ with the equality if and only if *G* is a complete multipartite graph. Here, m is the number of edges and $M_1(G)$ is the sum of squares of the vertex degrees of G. He also determined the extremal graphs with respect to the PI index among all complete multipartite graphs. He wrote: "we do not know whether K_n is the graph with the maximal PI index among all the simple connected graphs on n vertices". The aim of this paper is to present a new approach for studying such problems. As a consequence, a sequence $\{G_n\}_{n\geq 1}$ of graphs is presented such that $PI(G_n) \geq PI(K_n)$, for all $n \geq 1$.

Let G and H be simple graphs. The union $G \cup H$ of G and H is a graph with $V(G \cup H) = V(G) \cup V(H)$ and $E(G \cup H) = E(G) \cup E(H)$. The join 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 a graph with $V(G + H) = V(G) \cup V(H)$ and $E(G + H) = E(G) \cup E(H) \cup \{uv \mid u \in V(G) \ \& \ v \in V(H)\}$. For three or more disjoint graphs $G_1, G_2, \ldots, G_n$, the sequential join $G_1 + G_2 + \ldots + G_n$ is the graph $(G_1 + G_2) \cup (G_2 + G_3) \cup \ldots \cup (G_{n-1} + G_n)$. Obviously, if K_n shows a complete graph by n vertices then $K_n + K_m = K_{n+m}$.

For two vertices u and v of a graph G, the distance d(u,v) is defined as the length of a minimal path connecting them. Suppose $e = uv \in E(G)$ and $w \in V(G)$. Define $d(e,w) = Min\{d(u,w),d(v,w)\}$. If $f = ab \in E(G)$ then f is said to be parallel with e and write $f \parallel e$, if $d(e,a) = d(e,b)$. Now define $M_u(v)=\{f \in E(G) \mid d(f,v) < d(f,u)\}$ and $M_v(u)$ analogously. Set $m_u(v) = |M_u(v)|$ and $m_v(u) = |M_v(u)|$. It is easy to see that the parallelism is not generally symmetric.

In this paper, we only consider connected graphs. Our notation is standard and mainly taken from [15].

2. Results and Discussion

Suppose G is a simple graph with exactly m edges. In [5], the authors proved that $PI(G) \leq m(m - 1)$ with equality if and only if G is a tree or a cycle of odd length. Therefore, it is natural to ask about the order of magnitude for PI index with respect to the number of vertices.

Suppose n is given and i is a natural number such that $n \equiv i \pmod 4$. Define sequence $\{F_n\}_{n\geq 1}$ as follows:

$$F_n = K_{((n-i)/4)} + H_1 + H_2 + K_{((n-i)/4)+i},$$

where H_1 and H_2 are arbitrary graphs with exactly $(n-i)/4$ vertices, and K_m shows a complete graph with m vertices, Figure 1.

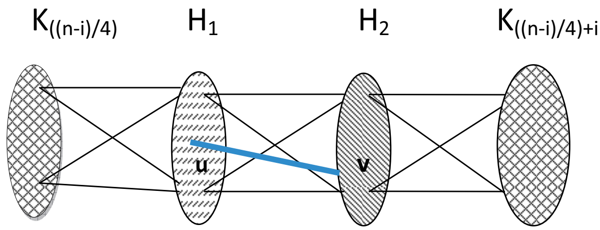

Figure 1. The Structure of the Graph F_n.

For every n, F_n has n vertices and for any edge $uv \in E(F_n)$ such that $u \in V(H_1)$ and $v \in V(H_2)$, $M_u(v) \cup M_v(u) \supseteq E(K_{((n-i)/4)+i}) \cup E(K_{((n-i)/4)})$. Notice that all of the vertices of $K_{((n-i)/4)}$ are closer to u than v and all of the vertices of $K_{((n-i)/4)+i}$ are closer to v than u. By the structure of F_n, the number of such edges between H_1 and H_2 in F_n is equal to $((n-i)/4)^2$. So

$$PI(F_n) > \left(\frac{n-i}{4}\right)^2 \left[\binom{\frac{n-i}{4}}{2} + \binom{\frac{n-i}{4}+i}{2}\right]$$

On the other hand $PI(K_n) = n(n-1)(n-2)$ and so

$$\lim_{n\to\infty} \frac{PI(F_n)}{PI(K_n)} = \infty.$$

Thus, we can find a sequence $\{G_n\}_{n>r}$ of graphs such that for some r, $PI(G_n) > PI(K_n)$, $n > r$.

Proposition. For any n-vertex graph G the inequality $PI(G) < \frac{n^4}{4}$ holds. On the other hand, there is a sequence of graphs $\{H_n\}_{n>0}$ such that H_n is an n vertices graph and

$$\lim_{n\to\infty} \frac{PI(H_n)}{n^4} > 0.$$

Proof. Suppose G is an n-vertex graph then for $e = uv \in E(G)$, $[m_u(v) + m_v(u)] \le |E(G)| - 1 \le \binom{n}{2} - 1$. Thus $PI(G) < \binom{n}{2}^2 < \frac{n^4}{4}$. Now consider $\{H_n\}_{n>0}$ to be a sequence of graphs with $H_n \cong F_n$, for each n. Then $\lim_{n\to\infty} \frac{PI(F_n)}{n^4} \ge \frac{1}{256}$, as desired. ▲

To construct a family of graphs $\{G_n\}$ with greater PI index than complete graphs, we consider a special case of F_n, i.e. $H_1 \cong K_{\frac{n-i}{4}} \cong H_2$. Suppose $a = (n - i)/4$. Then, for $uv \in E(G)$, we have:

$$[m_u(v) + m_v(u)] = \begin{cases} 2(a-2) + 2a & uv \in E(K_{\frac{n-i}{4}}) \\ 2(a+i-2) + 2a & uv \in E(K_{\frac{n-i}{4}+i}) \\ \binom{2a+i}{2} + a + 2(a-1) + 2(a-1) & u \in V(H_1);\ v \in V(K_{\frac{n-i}{4}}) \\ \binom{2a}{2} + 2(a+i-1) + 2(a-1) + a & u \in V(H_2), v \in V(K_{\frac{n-i}{4}+i}) \\ 2(a-2) + 4a & uv \in V(H_1) \\ 2(a-2) + 2(a+i) + 2a & uv \in V(H_2) \\ 2(a-1) + a + \binom{a}{2} + 2(a-1) + (a+i) + \binom{a+i}{2} & u \in V(H_1), v \in V(H_2) \end{cases}.$$

Since $|\{e \mid e=uv, u \in V(H_1), v \in V(H_2)\}| = |\{e \mid e=uv, u \in V(H_1), v \in V(K_{\frac{n-i}{4}})\}| = a^2$, $|\{e \mid e = uv, u \in V(H_2), v \in V(K_{\frac{n-i}{4}+i})\}| = a(a + i)$, $|E(K_a)| = |E(H_1)| = |E(H_2)| = \binom{a}{2}$ and $|E(K_{a+i})| = \binom{a+i}{2}$ then

$$PI(G_n) = \sum_{e=uv\in E(Gn)}[m_u(v) + m_v(u)]$$

$$= 2\binom{a}{2}[8a - 6 + i] + 2\binom{a+i}{2}[2a - 2 + i]$$

$$+a^2\left[2\binom{a}{2} + 2\binom{a+i}{2} + a(a+i) + 11a + i - 8\right]$$

$$+ a(a+i)\left[2\binom{a}{2} + a^2 + 5a + 2i - 4\right]$$

$$= 2i + 8a - 30a^2 - 12ai + 5a^3i + 12a^2i - 3i^2 + 6ai^2 + 5a^4$$

$$+ 23a^3 + i^3 + a^2i^2$$

$$= \frac{5}{256}n^4 + \frac{23}{64}n^3 + \frac{1}{256}(-480 - 84i - 14i^2)n^2$$

$$+ \frac{1}{256}(512 + 192i + 276i^2 + 8i^3)n + \frac{1}{256}i^2(i+12)(i-40).$$

Define F(n) = PI(Gₙ) − PI(Kₙ) = $\frac{5}{256}n^4 - \frac{41}{64}n^3 + \frac{9}{8}n^2 - \frac{21}{64}n^2 i - \frac{7}{128}n^2 i^2 + \frac{3}{4}n\,i + \frac{69}{64}n\,i^2 + \frac{1}{32}n\,i^3 + \frac{1}{256}i^4 - \frac{7}{64}i^3 - \frac{15}{8}i^2$. By elementary calculus, for n ≥ 32, F(n) > 0. In the following tables, the values of PI(F_n) and PI(K_n), 27≤ $n \le 40$, are computed.

Table 1. The Values of PI(Gn) and PI(Kn), 27 ≤ n ≤ 40.

n	PI(G_n)	PI(K_n)	n	PI(G_n)	PI(K_n)
27	15390	17350	**34**	37312	35904
28	18480	19656	**35**	41110	39270
29	20790	21924	**36**	47214	42840
30	23282	24360	**37**	51858	46620
31	25962	26970	**38**	56772	50616
32	30400	29760	**39**	61962	54834
33	33740	32736	**40**	70080	59280

We end this paper with the following conjecture:

Conjecture. For every sequence $\{L_n\}_{n\geq 1}$, $|V(L_n)| = n$, of simple connected graphs,

$$\lim_{n\to\infty} \frac{PI(L_n)}{n^4} \le \frac{3}{5^3}\ .$$

Moreover, the bound is sharp.

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