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Disproving a Conjecture on PI–Index of Graphs*

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Abstract

The PI-index of a graph G is defined by $\mathrm{PI}(G) = \sum_{e=uv\in E}(m_u(e) + m_v(e))$, where $m_u(e)$ is the number of edges in G lying closer to the vertex u than to the vertex v. In this paper, using probabilistic method we disprove a conjecture about the PI-index posed by Khalifeh et al. [Order of Magnitude of the PI index, MATCH Commun. Math. Comput. Chem. 65 (2011) 51–56].

1 Introduction

All graphs considered here are simple and undirected. For notations and terminologies used but not defined here, we refer to [1, 2].

A *topological index* is a real number related to a graph. It must be a structural invariant, i.e., it is preserved by every graph automorphism. Several topological indices have been defined and many of them have found applications as means for modeling chemical, pharmaceutical and other properties of molecules. We here focus on the so-called *PI-index* of graphs.

Let $G = (V(G), E(G))$ be a connected graph with order $n = |V(G)|$. As usual, the *distance* between the vertices u and v of G is denoted by $d(u, v)$ and it is defined as

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the number of edges in a minimal path connecting the vertices u and v. For an edge $e = xy \in E(G)$, we define the *edge-distance* of the edge e to a vertex $z \in V(G)$ as follows:

$$d(z, e) = \min\{d(z, x), d(z, y)\}.$$

For $e = uv \in E(G)$, let $E_u(e)$ be the subset of edges of $E(G)$ which are closer to u than v, and $E_v(e)$ be the subset of edges of $E(G)$ which are closer to v than u; More precisely,

$$E_u(e) = \{f \mid d(u, f) < d(f, v), f \in E(G)\} \quad \text{and} \quad E_v(e) = \{f \mid d(v, f) < d(f, u), f \in E(G)\}.$$

Set $m_u(e) = |E_u(e)|$ and $m_v(e) = |E_v(e)|$. Then, the *Padmakar-Ivan index* [7], abbreviated as PI-index, is defined as

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

About the PI-index, there are already many published papers on its mathematical properties [3, 8, 10, 11, 14, eg.], and on its applications to the chemical properties of molecules [5, 6, 12, 13, eg.]. For more results, the readers can search the realted papers online.

Although the background of PI-index comes from the chemistry, as a graph parameter it is an important topological index based on the distances in graphs. From this viewpoint, we will consider the order of magnitude of the PI-index, and disprove a nearly decade-old conjecture by the probabilistic method.

In 2011, Khalifeh, Yousefi-Azari and Ashrafi [9] not only constructed a sequence $\{G_n\}_{n\geq 1}$ of connected graphs such that $\lim_{n\to\infty} \frac{\mathrm{PI}(G_n)}{n^4} = \frac{5}{256}$, but put forward the following conjecture.

Conjecture 1. [9] *For every sequence $\{G_n\}_{n\geq 1}$, $|V(G_n)| = n$, of connected graphs,*

$$\lim_{n\to\infty} \frac{\mathrm{PI}(G_n)}{n_4} \leq \frac{3}{5^3}.$$

Moreover, the bound is sharp.

Note that $\frac{3}{5^3} = 0.024$. In next section, we firstly investigate the expectation of the PI-index of random graph $G(n, p)$, and then disprove the above conjecture. In Section 3, we give some remarks and propose two problems for future study.

2 Main results

Let n be a positive integer and $0 \leq p \leq 1$. The Gilbert random graph $G(n,p)$ is a probability space over the set of graphs on the vertex set $\{1,2,\ldots,n\}$ determined by

$$\Pr[\{i,j\} \in G] = p$$

with these events mutually independent [4].

Lemma 2.1. *The expectation of* PI *index of* $G(n,p)$ *is at least*

$$2\binom{n}{2}\binom{n-2}{2}p^3(1-p)^2(2-p).$$

Proof. Let u, v be any two vertices of $G(n,p)$. Clearly, there are $\binom{n}{2}$ such choices. Suppose $e = uv$ be an edge of $G(n,p)$. Let $m_u(e)$ and $m_v(e)$ be defined as in Section 1. We next compute $m_u(e)$ and $m_v(e)$.

Selecting two vertices $x, y \in V(G(n,p))\backslash\{u,v\}$, we have $\binom{n-2}{2}$ such choices. Note that xy has probability p of being an edge of $G(n,p)$. Assume that xy is an edge of $G(n,p)$. Firstly, we consider the case that the distance between the edge xy and u is less than the distance between the edge xy and v. We just consider that at least one vertex of $\{x,y\}$ is adjacent to u, and both vertices $\{x,y\}$ are not adjacent to v. Easily to obtain the probability that at least one vertex of $\{x,y\}$ is adjacent to u is $1-(1-p)^2 = p(2-p)$, and the probability that both vertices $\{x,y\}$ are not adjacent to v is $(1-p)^2$. Hence, the probability that at least one vertex of $\{x,y\}$ is adjacent to u and both vertices $\{x,y\}$ are not adjacent to v is $p(2-p)\cdot(1-p)^2$. Therefore,

$$m_u(e) \geq \binom{n-2}{2}p \cdot p(2-p)\cdot(1-p)^2 = \binom{n-2}{2}p^2(1-p)^2(2-p).$$

Similarly, we get $m_v(e) \geq \binom{n-2}{2}p^2(1-p)^2(2-p)$. So, the expectation of PI-index of $G(n,p)$ can be computed as follows:

$$\begin{aligned} E[\mathrm{PI}(G(n,p))] &\geq \binom{n}{2}p\left[\binom{n-2}{2}p^2(1-p)^2(2-p) + \binom{n-2}{2}p^2(1-p)^2(2-p)\right] \\ &= 2\binom{n}{2}\binom{n-2}{2}p^3(1-p)^2(2-p). \end{aligned}$$

This finishes the proof. ∎

We are now in the stage to disprove Conjecture 1.

Theorem 2.2. *For large enough n, there exists a graph H_n of order n such that the coefficient of n^4 in $\mathrm{PI}(H_n)$ is greater or equal to $\frac{587-143\sqrt{13}}{2916}$. In other words,*

$$\lim_{n\to\infty} \frac{\mathrm{PI}(H_n)}{n^4} \geq \frac{587-143\sqrt{13}}{2916} = 0.02448+ .$$

Consequently, Conjecture 1 invalidates.

Proof. Let $f(p) = p^3(1-p)^2(2-p)$ with $0 < p < 1$. A direct calculation shows that the derivative of $f(p)$ on p is

$$f'(p) = -6p^5 + 20p^4 - 20p^3 + 6p^2,$$

whose root belonging to the interval $(0,1)$ is $p = \frac{7-\sqrt{13}}{6}$. Thereby, the maximum value of $f(p)$ is $\frac{587-143\sqrt{13}}{1458}$. Since $2\binom{n}{2}\binom{n-2}{2} \sim \frac{1}{2}n^4$, by $p = \frac{7-\sqrt{13}}{6}$ we obtain

$$2\binom{n}{2}\binom{n-2}{2}p^3(1-p)^2(2-p) \sim \frac{587-143\sqrt{13}}{2916}n^4.$$

So, there exists a graph H_n of order n such that

$$\mathrm{PI}(H_n) \geq E[\mathrm{PI}(G(n,p))].$$

Due to $\frac{587-143\sqrt{13}}{2916} > \frac{3}{5^3}$, we conclude that Conjecture 1 is invalid.

The proof is completed. ■

3 Concluding remarks

In this paper, we mainly prove that the Conjecture 1 is incorrect. Nevertheless, we still do not know the maximum order of magnitude of the PI-indices of graphs. In the end, we pose the following two problems to finish this paper.

Problem 1. *Among all connected graphs of order n, find the the maximum order of magnitude of the PI-indices.*

Problem 2. *Construct a graph G of order n such that the coefficient of n^4 in $\mathrm{PI}(G)$ is at least $\frac{587-143\sqrt{13}}{2916}$.*

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