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On the PI index of a graph [1]

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Abstract

The PI index of a graph $G = (V, E)$ is defined as $PI(G) = \sum_{e \in E}(n_{eu}(e|G) + n_{ev}(e|G))$, where $e = uv$, $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u. In this paper, it is showed that $PI(G) \geq M_1(G) - 2|E|$ with the equality if and only if G is a complete multipartite graph, where $M_1(G) = \sum_{v \in V} d^2(v)$ is the first Zagreb index of G. Moreover, we determine the extremal graphs with respect to the PI index among all complete multipartite graphs.

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1 Introduction

A topological index is a real number related to a molecular graph and a structural invariant, i.e., it must not depend on the labeling or the pictorial representation of a graph. Many topological indices have been defined and several of them have found applications as means to model chemical, pharmaceutical and other properties of molecules

Here, we consider the Padmakar-Ivan index, which is abbreviated as the PI index [1,2]. The PI index is an edge-additive topological index introduced as a counterpart to the vertex-multiplicative Szeged index. Applications of the PI index to QSRP/QSAR were studied in [3]. The index was mostly compared with the Wiener and the Szeged index. It turned out that the PI index has similar discriminating power as the other two indices and in many cases it gives better result. The PI index is usually easier to compute than the Wiener and the Szeged indices and is a topological index worth studying. In a series of papers, Khadikar and coauthors [1-11] computed the PI index of some chemical graphs. In particular, John and Khadikar [11] described a method of computing PI index of benzenoid hydrocarbons using orthogonal cuts. The method requires the finding of number of edges in the orthogonal cuts in a benzenoid system. Klavžar [12] introduced the PI-partition and expressed the PI of a graph in terms of its PI-partition. Ashrafi and Loghman [13,14] computed the PI indices of armchairand zig-zag polyhex nanotubes. The present author [15] gave the formulas for calculating the PI indices of catacondensed hexagonal systems, and characterized the extremal catacondensed hexagonal systems with the minimum or maximum PI index; [16-19] computed the PI indices of $TUVC_6[2p, q]$, the torus and the nanotube covering by C_4 and C_8, and established a relation between the PI indices of a phenylene and of the corresponding hexagonal squeeze.

In this paper, we continue to study the PI index and show that $PI(G) \geq M_1(G) - 2|E|$ with the equality if and only if G is a complete multipartite graph, where $M_1(G) = \sum_{v \in V} d^2(v)$ is the first Zagreb index of G.

2 Preliminaries

Let G be a simple graph without directed, the vertex- and edge-sets of which are represented by V(G) and E(G), respectively. The graph G is said to be connected if for every pair of vertices u and v in $V(G)$ there exists a path between u and v. Here, we only consider connected graphs. If e is an edge of G connecting the vertices u and v, then we write $e = uv$. The number of

vertices of G is denoted by n. The distance between a pair of vertices u and v of G is denoted by $d(u,v)$. We now give the definition of the PI index of a graph G. Suppose that $e = uv$ is an edge of G, $n_{eu}(e|G)$ is the number of edges lying closer to vertex u than to vertex v and $n_{ev}(e|G)$ is the number of edges lying closer to vertex v than to vertex u. Then the PI index of a graph G is defined as:

$$PI(G) = \sum_{e \in E(G)} (n_{eu}(e|G) + n_{ev}(e|G)). \quad (1)$$

Edges equidistant from both ends of the edge $e = uv$ are not counted and the number of such edges is denoted by $c(e)$. To clarify this, for every vertex w and any edge $e = uv$ of graph G, we define $d(e,w) = \min\{d(u,w), d(v,w)\}$. Then e' is equidistant from both ends of the edge $e = uv$ if $d(e',u) = d(e',v)$.

Note that if G is bipartite, then $n_{eu}(e|G) = |E(G[V_u])|$ and $n_{ev}(e|G) = |E(G[V_v])|$ are the numbers of edges in the subgraphs of G induced by $V_u = \{x \in V(G) | d(x,u) < d(x,v)\}$ and $V_v = \{y \in V(G) | d(y,v) < d(y,u)\}$, respectively. But it is not true if G is not bipartite.

We denote the degree and the neighborhood of a vertex v by $d_G(v)$ and $N_G(v)$, respectively. Then $d_G(v) = |N_G(v)|$. The first Zagreb index M_1 and the second Zagreb index M_2 of G are defined as

$$M_1(G) = \sum_{v \in V(G)} d_G^2(v), \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$$

The Zagreb indices M_1 and M_2 were introduced in [20] and elaborated in [21]. The main properties of M_1 and M_2 were summarized in [22,23]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [24,25].

3 A lower bound for the PI index of a graph

We now give a lower bound for the PI index of a graph in terms of the first Zagreb index.

Theorem 1. Let $G = (V, E)$ be a simple connected graph with m edges. Then

$$PI(G) \geq M_1(G) - 2m$$

with the equality if and only if G is a complete multipartite graph.

Proof. Let $c(e)$ be the number of edges equidistant from both ends of the edge $e = uv$. Then $c(e) + n_{eu}(e|G) + n_{ev}(e|G) = m$. From the equation

(1), we have

$$PI(G) = m^2 - \sum_{e \in E(G)} c(e).$$

And,

$$1 \le c(e) \le m - (d_G(u) - 1) - (d_G(v) - 1) = m + 2 - d_G(u) - d_G(v).$$

So,

$$\begin{aligned} PI(G) &\ge m^2 - \sum_{e=uv \in E(G)} (m + 2 - d_G(u) - d_G(v)) \\ &= \sum_{e=uv \in E(G)} (d_G(u) + d_G(v)) - 2m \\ &= \sum_{v \in V(G)} d_G^2(v) - 2m = M_1(G) - 2m \end{aligned}$$

with the equality if and only if

$$c(e) = m + 2 - d_G(u) - d_G(v) \tag{2}$$

for all edges $e = uv$ of G.

In the following, we prove that the equation (2) holds if and only if G is a complete multipartite graph.

Let $N_G(u) \cap N_G(v) = \{z_1, z_2, \cdots, z_r\}$, $N_G(u) - \{v\} - N_G(v) = \{x_1, x_2, \cdots, x_s\}$, $N_G(v) - \{u\} - N_G(u) = \{y_1, y_2, \cdots, y_t\}$, as shown in Figure 1.

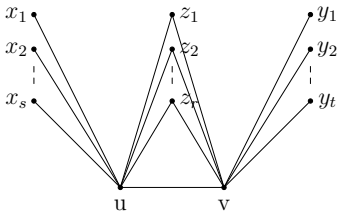

Figure 1.

Claim 1. $x_i z_j, x_i y_k, y_k z_j \in E(G)$, $1 \le i \le s$, $1 \le j \le r$, $1 \le k \le t$.

If $x_i z_j \notin E(G)$, then $d(u, z_j v) = 1$ and $d(x_i, z_j v) > 1$ since $x_i v \notin E(G)$. So, $z_j v \notin C(ux_i) = \{f | f$ is equidistant from both ends of the edge $ux_i\}$, and $c(ux_i) < m + 2 - d_G(u) - d_G(x_i)$, contradicting to the equation (2).

Similarly, we have $x_iy_k, y_kz_j \in E(G)$.

Claim 2. $x_ix_j \notin E(G)$, $y_iy_j \notin E(G)$.

If $x_ix_j \in E(G)$, then $d(u, x_ix_j) = 1$ and $d(v, x_ix_j) = 2$ since $x_iv \notin E(G)$ and $x_jv \notin E(G)$. So, $c(uv) < m + 2 - d_G(u) - d_G(v)$, contradicting to the equation (2).

Similarly, $y_iy_j \notin E(G)$.

Claim 3. The subgraph $G[z_1, z_2, \cdots, z_r]$ induced by $\{z_1, z_2, \cdots, z_r\}$ is a complete multipartite graph.

This only needs to show that $z_jz_k \in E(G)$ if $z_iz_j \notin E(G)$ and $z_iz_k \in E(G)$ for any three different vertices $z_i, z_j, z_k \in \{z_1, z_2, \cdots, z_r\}$.

Suppose that $z_jz_k \notin E(G)$, then $d(u, z_iz_k) = 1$ and $d(z_j, z_iz_k) = 2$. So, $c(uz_j) < m + 2 - d_G(u) - d_G(z_j)$, contradicting to the equation (2).

By the claims 1-3, G is a complete multipartite graph.

Conversely, it is obvious that $c(e) = m + 2 - d_G(u) - d_G(v)$ for all edges $e = uv$ of a complete multipartite graph G. □

In particularly, we have

Corollary 2. If $G = (V, E)$ is a simple connected K_3-free graph with m edges, then

$$PI(G) \geq M_1(G) - 2m$$

with the equality if and only if G is a complete bipartite graph.

Note that the cocktail-party graph (or hyperoctahedral graph) $CP(s)$, obtained by removing s disjoint edges from the complete graph K_{2s}, is a complete multipartite graph, and its PI index is

$$PI(CP(s)) = M_1(CP(s)) - 2|E(CP(s))| = 4s(s-1)(2s-3).$$

4 The PI indices of complete multipartite graphs

In this section, we characterize the complete multipartite graphs with the extremal PI indices.

A p-partite graph is one whose vertex set can be partitioned into p subsets so that no edge has both ends in any one subset; a complete p-partite graph is one that is simple and in which each vertex is joined to every vertex that is not in the same subset.

When $p \geq 2$, we write $K_{n_1,n_2,\cdots,n_p}$ for the complete p-partite graph with partite subsets of sizes $n_1, n_2, \cdots, n_p$.

The complete p-partite graph on n vertices in which each part has either $[n/p]$ or $\{n/p\}$ vertices is denoted by $T_{n,p}$, where $[x]$ denotes the largest integer no more than x and $\{x\}$ denotes the smallest integer no less than x.

Theorem 3. Let G be a complete p-partite graph on n vertices. Then

(i) $PI(G) \leq PI(T_{n,p})$ with the equality if and only if G is isomorphic to $T_{n,p}$, i.e., $T_{n,p}$ is the unique graph with the maximal PI index among all complete p-partite graphs on n vertices;

(ii) $PI(G) \geq PI(K_{1,\cdots,1,n-p+1})$ with the equality if and only if G is isomorphic to $K_{1,\cdots,1,n-p+1}$, i.e., $K_{1,\cdots,1,n-p+1}$ is the unique graph with the minimal PI index among all complete p-partite graphs on n vertices;

Proof. Let $G = K_{n_1,n_2,\cdots,n_p}$ be a complete p-partite graph on n vertices.

(i) If G is not isomorphic to $T_{n,p}$, then there are $1 \leq i, j \leq p$ such that $n_i - n_j \geq 2$. Let $G' = K_{n_1,\cdots,n_i-1,\cdots,n_j+1,\cdots,n_p}$ be the complete p-partite graph on n with partite subsets of sizes $n_1, \cdots, n_{i-1}, n_i - 1, n_{i+1}, \cdots, n_{j-1}, n_j + 1, n_{j+1}, \cdots, n_p$.

From Theorem 1, we have

$$PI(G) = M_1(G) - 2|E(G)| = \sum_{k=1}^{p} n_k(n-n_k)^2 - \sum_{k=1}^{p} n_k(n-n_k),$$

and

$$\begin{aligned} & PI(G') - PI(G) \\ = \; & (n_i-1)(n-n_i+1)^2 + (n_j+1)(n-n_j-1)^2 - (n_i-1)(n-n_i+1) \\ & -(n_j+1)(n-n_j-1) - n_i(n-n_i)^2 - n_j(n-n_j)^2 \\ & +n_i(n-n_i) + n_j(n-n_j) \\ = \; & (n_i-n_j-1)(4n-3n_i-3n_j-2) > 0. \end{aligned}$$

That is, if G is not isomorphic to $T_{n,p}$, there is a complete p-partite graph G' on n vertices such that $PI(G') > PI(G)$. So, $T_{n,p}$ is the unique graph with the maximal PI index among all complete p-partite graphs on n vertices.

(ii) Without loss of the generality, we assume that $n_1 \leq n_2 \leq \cdots \leq n_p$. If G is not isomorphic to $K_{1,\cdots,1,n-p+1}$, then there are $1 \leq i < p$ such that $n_1 = \cdots = n_{i-1} = 1$ and $n_i \geq 2$. By the proof of (i), we have $PI(G) > PI(G'')$, where $G'' = K_{1,\cdots,1,n_i-1,\cdots,n_p+1}$ is the complete p-partite graph on n with partite subsets of sizes $1, \cdots, 1, n_i - 1, n_{i+1}, \cdots, n_{p-1}, n_p + 1$. So, $K_{1,\cdots,1,n-p+1}$ is the unique graph with the minimal PI index among all complete p-partite graphs on n vertices. □

If $d_1 \leq d_2 \leq \cdots \leq d_n$ is the degree sequence of a complete multipartite

graph G on n vertices, then by Theorem 1, we have

$$PI(G) = M_1(G) - 2|E(G)| = \sum_{i=1}^{n}(d_i^2 - d_i) = \sum_{i=1}^{n}(d_i - \frac{1}{2})^2 - \frac{1}{4}n \qquad (3)$$

Let $d_1 \leq d_2 \leq \cdots \leq d_n$ and $d'_1 \leq d'_2 \leq \cdots \leq d'_n$ be the degree sequences of $T_{n,p}$ and $T_{n,p+1}$, respectively. Then $d_i \leq d'_i$, $1 \leq i \leq n$ and at least one of these inequalities is strict. By the equation (3),

$$PI(T_{n,p}) < PI(T_{n,p+1}).$$

Similarly, $PI(K_{1,\cdots,1,n-p+1}) < PI(K_{1,\cdots,1,n-p})$.
So, we have

Theorem 4. (i) The complete graph $K_n = K_{1,1,\cdots,1}$ is the unique graph with the maximal PI index among all the complete multipartite graphs on n vertices;
(ii) The star graph $K_{1,n-1}$ is the unique graph with the minimal PI index among all the complete multipartite graphs on n vertices. □

Since every tree with n vertices has the same PI index and $K_{1,n-1}$ is a tree with n vertices, we prove the following result from Theorem 1 and Theorem 4(ii).

Corollary 5. Let G be a simple connected graph with n vertices. Then $PI(G) \geq (n-1)(n-2)$ with the equality if and only if G is a tree. □

From Theorem 4(i), $K_n = K_{1,1,\cdots,1}$ is the unique graph with the maximal PI index among all the complete multipartite graphs on n vertices. But we do not know whether K_n is the graph with the maximal PI index among all the simple connected graphs on n vertices. So, we end this paper with the following problem.

Problem. Characterize the graph(s) on n vertices with the maximal PI index.

References

[1] P. V. Khadikar, On novel structural descriptor PI, *Nat. Sci. Lett. 23*, (2000), 113-118.

[2] P. V. Khadikar, S. Karmarkar and V. K. Agrawal, Relationships and relative correlation potential of the Wiener, Szeged and PI indices, *Nat. Sci. Lett. 23*, (2000), 165-170.

[3] P. V. Khadikar, S. Karmarkar and V. K. Agrawal, A novel PI index and its applications to QSRP/QSAR studies, *J. Chem. Inf. Comput. Sci. 41*, (2001), 934-949.

[4] P. V. Khadikar, P. P. Kale, N. V. Deshpande, S. Karmarkar and V. K. Agrawal, Novel PI indices of hexagonal chains, *J. Math. Chem. 29*, (2001), 143-150.

[5] S. Singh, S. Joshi, A. Shrivastava and P.V. Khadikar, A novel method for estimating motor octane number (MON) C a structure-property relationship approach, *J. Sci. Ind. Res. 61*, (2002), 961-965.

[6] P. V. Khadikar, S. Karmarkar, S. Singh and A. Shrivastava, Use of the PI index in predicting toxicity of nitrobenzene derivatives, *Bioorg. Med. Chem. 10*, (2002), 3163-3170.

[7] P. V. Khadikar, A. Phadnis and A. Shrivastava, QSAR study on toxicity to aqueous organism using PI index, *Bioorg. Med. Chem. 10*, (2002), 1181-1188.

[8] P. V. Khadikar, D. Mandloi, A.V. Bajaj and S. Joshi, QSAR study on solubility of alkanes in water and their partition coefficients in different solvent system using PI index, *Bioorg. Med. Chem. Lett. 13*, (2003), 419-422.

[9] M. Jaiswal and P. V. Khadikar, QSAR study on tadpole narcosis using PI index: a case of heterogeneous set of compounds, *Bioorg. Med. Chem. 12*, (2004), 1731-1736.

[10] P. V. Khadikar, D. Mandloi and A. V. Bajaj, Novel applications of PI index in estimating organic reactivity-: CH: Acidity, s-Character and steric Energes, *Oxid. Commun., 27*, (2004), 23-28.

[11] P. E. John, P. V. Khadikar, A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts, *J. Math. Chem. 42*, (2007), 37-45.

[12] S. Klavžar, On the PI index: PI-partitions and cartestian product graphs, *MATCH Commun. Math. Comput. Chem. 57*, (2007), 573-586.

[13] A. R. Ashrafi and A. Loghman, PI index of zig-zag polyhex nanotubes, *MATCH Commun. Math. Comput. Chem. 55*, (2006), 447-452.

[14] A. R. Ashrafi and A. Loghman, PI index of armchair polyhex nanotubes, *Ars Combin. 80*, (2006), 193-199.

[15] H. Deng, Extremal catacondensed hexagonal systems with respect to the PI index, *MATCH Commun. Math. Comput. Chem. 55*, (2006), 453-460.

[16] H. Deng, The PI index of $TUVC_6[2p; q]$, *MATCH Commun. Math. Comput. Chem., 55*, (2006), 461-476.

[17] L. Xu, H. Deng, PI indices of tori $T_{p,q}[C_4, C_8]$ covering by C_4 and C_8, *MATCH Commun. Math. Comput. Chem., 57*, (2007), 485-502.

[18] H. Deng, J. Hou, PI indices of nanotubes $SC_4C_8[q, 2p]$ covering by C_4 and C_8, *MATCH Commun. Math. Comput. Chem., 57*, (2007), 503-516.

[19] H. Deng, S. Chen, J. Zhang, The PI index of Phenylenes, *J. Math. Chem. 41*, (2007), 63-69.

[20] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett. 17*, (1972), 535-538.

[21] I. Gutman, B. Ruščić, N. Trinajstić,C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys. 62*, (1975), 3399-3405.

[22] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta 76*, (2003), 113-124.

[23] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem. 50*, (2004), 83-92.

[24] A. T. Balaban, I. Motoc, D.Bonchev, O. Mekenyan, Topological indices for structure-activity corrections, *Topics Curr. Chem. 114*, (1983), 21-55.

[25] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.