MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 123-130

ISSN 0340 - 6253

Sharp Bounds on the PI and Vertex PI Energy of Graphs

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(Received May 22, 2009)

Abstract

In this paper, the notions of PI and vertex PI energy of a graph G are introduced. They are defined as the sum of the absolute values of PI and vertex PI eigenvalues of G, respectively. In this paper, formulas for the PI and vertex PI energy of the Cartesian product of graphs are given. Some bounds for these quantities are also proved.

1. Introduction

Let G be a 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 $d_G(u,v)$ (d(u,v) for short) and it is defined as the number of edges in a shortest path connecting the vertices u and v.

Suppose *Graph* denotes the class of all graphs. A map *Top* from *Graphs* into real numbers is called a *topological index*, if G ≅ H implies that Top(G) = Top(H). The *Wiener index* was the first reported topological index based on graph distances [15]. This index is defined as the sum of all distances between vertices of the graph under consideration. We encourage the readers to consult papers [5,6] for background material as well as basic computational techniques related to the Wiener index.

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. The edge variants of $n_u(e)$ and $n_v(e)$ are denoted by $m_u(v)$ and $m_v(e)$, respectively. We now define four topological indices of the PI, vertex PI, Szeged and edge Szeged indices of the graph G as follows:

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

$$PI_v(G) = \sum_{e=uv} [n_u(e) + n_v(e)]$$

$$Sz(G) = \sum_{e=uv} n_u(e).n_v(e)$$

$$Sz_{e(G)} = \sum_{e=uv} m_u(e).m_v(e)$$

This topological indices attracted recently much attention [1,2,4,8,10-12,14]. The vertex PI matrix VPIM(G) of G is defined so that its (i,j)-entry, a_{ij}, is equal to

$$a_{ij} = \begin{cases} n_{v_i}(e) + n_{v_j}(e) & e = v_i v_j \\ 0 & otherwise \end{cases}.$$

The PI-matrix PIM(G) of G is defined analogously. In this paper, we discuss about vertex PI matrix. Similarly, these conclusions are established for the PI matrix. The eigenvalues of VPIM(G) are said to be the vertex PI-eigenvalues of G and form the VPIM(G)-spectrum of G, denoted by VPI-Spec(G).

Since the vertex PI-matrix is symmetric, all of its eigenvalues, δ_i, i = 1, 2, ..., n, are real and can be labeled so that $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$. If $\delta_{i1} > \delta_{i2} > \cdots > \delta_{ik}$ are distinct VPIM-eigenvalues, then the VPI-spectrum can be written as

$$\mathrm{VPI-Spec(G)} = \begin{pmatrix} \delta_{i1} & \delta_{i2} & \dots & \delta_{ik} \\ m_1 & m_2 & \dots & m_k \end{pmatrix},$$

where m_j indicates the algebraic multiplicity of the eigenvalue δ_{ij}. Clearly, $m_1 + m_2 + \cdots + m_k = n$. The ordinary spectrum of G, which is the spectrum of the adjacency matrix of G is well studied and many properties of graphs in connection with the spectrum are revealed during the past years. The notion of the energy of a graph was introduced by Ivan Gutman [7, 9]. It is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. In a similar way, the vertex PI energy of a graph G, $VPIE(G) = \sum_{i=1}^{n} |\delta_i|$, is defined.

In this paper, some bounds for the PI and vertex PI energy of graphs and its relationship with some topological indices are obtained.

2. Main Results

In this section, some bounds for the vertex PI-energy of graphs are obtained.

Theorem 1. Suppose G_1, G_2, …, G_s are connected graphs with n_1, n_2, …, n_s vertices, respectively. The VPI eigenvalues of $G = G_1 \times G_2 \times \ldots \times G_s$ are as follows:

$$\delta_{i_1,i_2,\ldots,i_s} = \left(\prod_{t=1}^{s} |G_t|\right)\sum_{j=1}^{s} \frac{\delta_{i_j}(G_j)}{|G_j|}, \qquad 1 \le i_j \le n_j, 1 \le j \le s.$$

In particular, if $H = G_1 = G_2 = \ldots = G_s$ then $\delta_{i_1,i_2,\ldots,i_s} = |H|^{s-1}\sum_{j=1}^{s}\delta_{i_j}(H)$ and zero is an eigenvalue of H^n, for $n = |H|$.

Proof. We first suppose $s = 2$, $G = G_1$ and $H = G_2$. If $(a,b)(x,y)$ is an edge of $G \times H$ then by definition $a = x$ and $by \in E(H)$ or $ax \in E(G)$ and $b = y$. Therefore, $n_{(a,b)}((a,\mathrm{b})(a,\mathrm{c})) = |G|n_b(bc)$ and $n_{(a,b)}((a,\mathrm{b})(x,\mathrm{b})) = |H|n_a(ax)$. So, $n_{(a,b)}\big((a,\mathrm{b})(a,\mathrm{c})\big) + n_{(a,c)}((a,\mathrm{b})(a,\mathrm{c})) = |G|(n_b(bc) + n_c(bc))$. On the other hand, $\mathrm{VPIM}(G \times H) = \mathrm{I}_{|\mathrm{H}|}\otimes|\mathrm{H}|.\mathrm{VPIM}(\mathrm{G}) + |\mathrm{G}|.VPIM(H)\otimes I_{|G|}$. This implies that $VPI - Spec(G \times H) = \{|H|\delta_i(G) + |G|\delta_j(H)\ |1 \le i \le |G|, 1 \le j \le |H|\}$. To deduce the result, it is enough to notice that $G_1 \times G_2 \times \ldots \times G_s = (G_1 \times G_2 \times \ldots \times G_{s-1}) \times G_s$ and apply an inductive argument. To prove the second part, we note that $\delta_{1,2,\ldots,n} = 0$ which proves our theorem. □

Corollary 1. With notation of Theorem 1, we have:

$$\mathrm{VPIE(G)} \le \prod_{\mathrm{t=1}}^{\mathrm{s}}(|\mathrm{G_t}|)^2 \sum_{\mathrm{j=1}}^{\mathrm{s}} \frac{\mathrm{VPIE(G_j)}}{|\mathrm{G_j}|^2}, 1 \le \mathrm{j} \le \mathrm{s}$$

with equality if and only if at most one of the graphs G_1, …, G_s are non-empty.

Proof. Apply Theorem 1. □

Lemma 1. Let G be n-vertex graph and $\mathrm{VPI - Spec(G)} = \{\delta_1, \delta_2, \ldots, \delta_n\}$. Then

$$\sum_{i=1}^{n} {\delta_i}^2 \le Min\,\{2PI_v(G)^2, 2nPI_v(G), 4(n-1)^2m + 4Sz(G), 2(n-1)PI_v(G) + 4Sz(G)\}\,.$$

Proof. Suppose $S = \sum_{i=1}^{n} {\delta_i}^2$. To prove the lemma, it is enough to show that $S \le 2PI_v(G)^2$, $S \le 2(n-1)PI_v(G)$ and $S \le 4(n-1)^2m + 8Sz(G)$. It is clear that

$$S = (\sum_{i=1}^{n} \delta_i)^2 - 2\sum_{i<j} \delta_i \, \delta_j = -2\sum_{i<j} \delta_i \delta_j$$

and by [3, Proposition 2.3], $c_2 = \sum_{i<j} \delta_i \delta_j$. Therefore

$$S = 2\sum_{i<j} (n_{v_i} + n_{v_j})^2 \leq 2PI_v(G)^2.$$

On the other hand,

$$S = 2\sum_{i<j} (n_{v_i} + n_{v_j})^2 \leq 2(n-1)\sum_{i<j} (n_{v_i} + n_{v_j}) \leq 2(n-1)PI_v(G),$$

$$S = 2\sum_{i<j} (n_{v_i} + n_{v_j})^2 = 2\sum_{i<j} ({n_{v_i}}^2 + 2n_{v_i}n_{v_j} + {n_{v_j}}^2) \leq 2(n-1)^2 m + 4Sz(G),$$

$$S = \sum_{i<j} (n_{v_i} + n_{v_j})^2 = 2\sum_{i<j} ({n_{v_i}}^2 + 2n_{v_i}n_{v_j} + {n_{v_j}}^2) \leq 2(n-1)PI_v(G) + 4Sz(G).$$

This completes our proof. □

Lemma 2. Let $\mathrm{VPI} - \mathrm{Spec(G)} = \{\delta_1, \delta_2, \ldots, \delta_n\}$, where $\delta_1 \leq \delta_2 \leq \cdots \leq \delta_n$. Then

$$\delta_n \leq Min\{\sqrt{\tfrac{2(n-1)}{n}} PI_v(G), \sqrt{\tfrac{2(n-1)}{n}}\sqrt{[(n-1)PI_v(G) + 2Sz(G)]}, \sqrt{\tfrac{(n-1)}{n}}\sqrt{[4m(n-1)^2 + 4Sz(G)}\}$$

Proof. Since $\sum_{i=1}^{n} \delta_i = 0$, $\delta_n = \sum_{i=1}^{n-1} \delta_i$. Therefore, $|\delta_n| \leq \sum_{i=1}^{n-1} |\delta_i| \leq \sqrt{n-1}\sqrt{\sum_{i=1}^{n-1} {\delta_i}^2}$ and so ${\delta_n}^2 \leq (n-1)\sum_{i=1}^{n-1} {\delta_i}^2 = (n-1)\left[\sum_{i=1}^{n} [{\delta_i}^2 - {\delta_n}^2\right]$. Therefore, ${\delta_n}^2 \leq \frac{(n-1)}{n}\sum_{i=1}^{n} {\delta_i}^2$. Now it is enough to apply Lemma 1 to complete the lemma. □

Theorem 2. Let G be a connected graph. Then $\mathrm{VPIE(G)} \leq \sqrt{2n\sum_{e=uv}(n_u + n_v)^2}$. Upper bound is achieved if and only if G is a trivial graph. Moreover, $\mathrm{VPIE(G)} \leq \sqrt{n\alpha}$, in which

$$\alpha = Min\{2PI_v(G)^2, 2(n-1)PI_v(G), 4(n-1)^{2m} + 4Sz(G), 2(n-1)PI_v(G) + 4Sz(G)\}.$$

Proof. By definition and Lemma 1,

$$\mathrm{V}PIE(G) = \sum_{i=1}^{n} |\delta_i| \leq \sqrt{n\sum_{i=1}^{n} {\delta_i}^2} = \sqrt{2n\sum_{e=uv\epsilon E(G)} [n_u(e) + n_v(e)]^2},$$

$$VPIE(G) \leq \sqrt{n}\sqrt{2PI_v(G)^2} = \sqrt{2n}PI_v(G)$$

$$VPIE(G) \leq \sqrt{n}\sqrt{2(n-1)PI_v(G)} = \sqrt{2n(n-1)PI_v(G)},$$

$$VPIE(G) \leq \sqrt{n}\sqrt{4(n-1)^2 m + 4Sz(G)} = 2\sqrt{n}\sqrt{2(n-1)^2 m + Sz(G)},$$

which completes our theorem. □

Lemma 3. Suppose G is bipartite graph with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and vertex PI eigenvalues of $\delta_1 \leq \cdots \leq \delta_n$. Then $VPIM(G) = nA(G)$ and $\delta_i = n\lambda_i, 1 \leq i \leq n$.

Proof. Suppose G is bipartite. Since G does not have odd cycles, $\mathrm{n_u(e)+n_v(e)=n}$, for edge e = uv. Therefore, $VPIM(G) = nA(G)$.

Corollary 2. If G is bipartite then $\det(\mathrm{VPIM(G)}) = n^n \det(A(G))$ and $n^2 \sqrt[n]{\det(A)} \leq VPIE(G) \leq n\sqrt{2mn}$.

Let G be a graph with V(G) = {v_1, v_2, ..., v_n} and vertex PI-matrix P. Then the vertex PI degree of v_i, denoted by P_i is given by $P_i = \sum_{j=1}^{n} a_{ij}$. Let the vertex PI degree sequence be {P_1,P_2, . . . , P_n}. Then the second vertex PI degree of v_i, denoted by T_i is given by $T_i = \sum_{j=1}^{n} a_{ij}P_j$. If {$P_1$,$P_2$, . . . , P_n} is the PI- degree sequence then G is k-vertex PI regular if P_i = k for all i. If G has the vertex PI-degree sequence {P_1, P_2, ..., P_n} and second vertex PI degree degree sequence {T_1, T_2, . . . , T_n} then G is pseudo k-vertex PI degree regular if $\frac{T_i}{P_i} = k$ for all i.

Theorem 3 ([13]). Suppose G is a graph, d = diam(G) and t = t(G) is the number of distinct eigenvalues of G. Then $t \leq d+1$. In particular, t(G) = 2 if and only if G is Complete. Moreover, if G has the vertex PI degree sequence $\{\mathrm{P_1, P_2, \dots, P_n}\}$ and second vertex PI degree sequence $\{\mathrm{T_1, T_2, \dots, T_n}\}$. Then

$$\delta_1 \geq \sqrt{\frac{\mathrm{T_1}^2 + \mathrm{T_2}^2 + \dots + \mathrm{T_n}^2}{\mathrm{P_1}^2 + \mathrm{P_2}^2 + \dots + \mathrm{P_n}^2}}.$$

Equality holds if and only if G is pseudo vertex PI regular.

Theorem 5. With the notations described above

$$VPIE(G) \leq \sqrt{\frac{\sum_{i=1}^{n} T_i^2}{\sum_{i=1}^{n} P_i^2}} + (n-1)\sqrt{S - \frac{\sum_{i=1}^{n} T_i^2}{\sum_{i=1}^{n} P_i^2}}$$

where S is the sum of the squares of entries in the vertex PI matrix. Equality holds if and only if either G is a complete graph or a pseudo k-vertex PI regular graph with three distinct eigenvalue $(k, \sqrt{\frac{S-k^2}{p-1}}, -\sqrt{\frac{S-k^2}{p-1}})$.

Proof. Let {δ_1,δ_2, . . . , δ_n} be the eigenvalues of G. Then

$$\sum_{i=1}^{n} \delta_i = 0 \qquad , \qquad \sum_{i=1}^{n} \delta_i^2 = S = \sum_{i,j=1}^{n} (a_{ij})^2$$

Now applying the Cauchy–Schwartz inequality to the two $n-1$ vectors (1, 1, . . ., 1) and ($|\delta_2|, |\delta_3|, \ldots, |\delta_n|$) we get,

$$(VPIE(G)-\delta_1)^2 \leq (n-1)(S-{\delta_1}^2)$$

Thus

$$VPIE(G) \leq \delta_1 + \sqrt{(n-1)(S-{\delta_1}^2)}$$

Define a function $f(x) = x + \sqrt{(n-1)(S-x^2)}$ for $\frac{2PI_v}{n} \leq x \leq \sqrt{S}$. Then by applying the max–min techniques of calculus we can see that $f(x)$ is monotonically decreasing in $x \geq \sqrt{\frac{S}{n}}$.

Now by Cauchy–Schwartz inequality we have

$${P_i}^2 = (\sum_{j=1}^{n} a_{ij})^2 \leq n\sum_{j=1}^{n} {a_{ij}}^2$$

Then

$$\sum_{i=1}^{n} {P_i}^2 \leq \sum_{i=1}^{n} n\sum_{j=1}^{n} {a_{ij}}^2 = n\sum_{i=1}^{n}\sum_{j=1}^{n} {a_{ij}}^2 = nS$$

Also $T_i = \sum_{j=1}^{n} a_{ij} P_j \geq \sum_{j=1}^{n} {a_{ij}}^2$ and $\sum_{i=1}^{n} T_i^2 \geq \sum_{i=1}^{n}(\sum_{j=1}^{n} {a_{ij}}^2)^2 \geq S^2$. Hence $\delta_i \geq \sqrt{\frac{\sum_{i=1}^{n} T_i^2}{\sum_{i=1}^{n} P_i^2}} \geq \sqrt{\frac{S^2}{nS}} = \sqrt{\frac{S}{n}}$. Therefore $VPIE(G) \leq f(\delta_1) \leq f(\sqrt{\frac{\sum_{i=1}^{n} T_i^2}{\sum_{i=1}^{n} P_i^2}})$ and thus the theorem is proved. We now suppose the equality holds. Then

$$\delta_1 = \sqrt{\frac{\sum_{i=1}^{n} T_i^2}{\sum_{i=1}^{n} P_i^2}}$$

and by Theorem 4 we have G is pseudo k-vertex PI regular. Also equality holds in the Cauchy–Schwartz inequality. Hence $|\delta_2| = |\delta_3| = \cdots = |\delta_n|$ and so $(\sum_{i=2}^{n}|\delta_i|)^2 = (n-1)(S-{\delta_1}^2)$. Hence $|\delta_i| = \sqrt{\frac{S-{\delta_1}^2}{n-1}}$, $i = 2,3,\ldots,n$. Since $|\delta_i| = \sqrt{\frac{S-{\delta_1}^2}{n-1}}$, δ_i can have at most two distinct values and we arrive at the following.

- G has exactly one eigenvalue. Then all eigenvalues are zero as the sum of eigenvalues is the trace of P and as G is connected. So, $G = K_1$.
- G has exactly two distinct eigenvalues. Then by Theorem 3, G is complete.

• G has exactly three distinct eigenvalues. Then $\delta_1 = \sqrt{\frac{\sum_{i=1}^{n} T_i^2}{\sum_{i=1}^{n} P_i^2}}$ and $|\delta_i| = \sqrt{\frac{S-{\delta_1}^2}{n-1}}$, $i = 2,3,\ldots,n$. Also $\frac{T_i}{P_i} = k$ for all i. Then we get G as a graph with three distinct eigenvalues $(k, \sqrt{\frac{S-k^2}{p-1}}, -\sqrt{\frac{S-k^2}{p-1}})$, proving the result. □

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