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On the Co-PI Spectral Radius and the Co-PI Energy of Graphs

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Abstract

The Co-PI eigenvalues of a connected graph G are the eigenvalues of its Co-PI matrix. In this study, Co-PI energy of a graph is defined as the sum of the absolute values of Co-PI eigenvalues of G. We also give some bounds for the Co-PI spectral radius and the Co-PI energy of graphs.

1 Introduction

Let G be a finite, connected, simple graph with $n = |V|$ vertices and $m = |E|$ edges. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between u and v in G. The diameter $diam(G)$ is the greatest distance between two vertices of G.

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The degree $\deg_G(v)$ of a vertex v is the number of edges incident with it in G. Let $e = uv$ be an edge connecting vertices u and v in G. Define the sets:

$$\begin{aligned} N_u(e) &= \{z \in V \,|d_G(z,u) < d_G(z,v)\} \\ N_v(e) &= \{z \in V \,|d_G(z,v) < d_G(z,u)\} \end{aligned}$$

which are sets consisting of vertices lying closer to u than to v and those lying closer to v than to u, respectively. The number of such vertices are denoted by

$$n_u = n_u(e) = |N_u(e)| \quad \text{and} \quad n_v = n_v(e) = |N_v(e)|.$$

Other terminology and notations neded will be introduced as it naturally occurs in the following and we use [1–3, 12] for those not defined here.

A topological index is a number related to graph which is invariant under graph isomorphism. In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modeling physicochemical, pharmacologic, toxicologic, biological and other properties of chemical compounds [7]. There exist several types of such indices, especially those based on vertex and edge distances. One of the most intensively studied topological indices is the Wiener index W, defined as the sum of distances between all pairs of vertices of the molecular graph [21].

Recently, Hassani et al. introduced a new topological index similar to the vertex version of PI index [11] . This index is called the Co-PI index of G and defined as:

$$Co - PI_v(G) = \sum_{e=uv\in E(G)} |n_u(e) - n_v(e)|.$$

Here the summation goes over all edges of G.

Fath-Tabar et al. proposed the Szeged matrix and Laplacian Szeged matrix in [5]. Then Su et al. introduced the Co-PI matrix of a graph [20]. The adjacent matrix $A(G) = [a_{ij}]_{n\times n}$ of G is the integer matrix with rows and columns indexed by its vertices, such that the $ij-$th-entry is equal to the number of edges connecting i and j. Let the weight of the edge $e = uv$ be a non-negative integer $|n_u(e) - n_v(e)|$, we can define a weight function: $w : E \to R^+ \cup \{0\}$ on E, which is said to be the $Co - PI$ *weighting* of G. The adjacency matrix of G weighted by the Co-PI weighting is said to be its $Co - PI$ *matrix* and denoted by $M_{CPI}(G) = [c_{ij}]_{n\times n}$ .That is,

$$c_{ij} = \begin{cases} |n_{v_i}(e) - n_{v_j}(e)|, & e = v_iv_j \\ 0 & ,otherwise \end{cases}.$$

Since Co-PI matrix is symmetric, all its eigenvalues $\lambda_i^*(G)$, $k = 1, 2, ..., |V|$, are real and can be labeled so that $\lambda_1^*(G) \geq \lambda_2^*(G) \geq ... \geq \lambda_n^*(G)$. The eigenvalues of M_{CPI} are said to be the Co-PI eigenvalues of G and the $M_{CPI}-$spectrum of G is denoted by Co-PI-Spec(G). The greatest eigenvalue λ_1^* will be called the Co-PI spectral radius of G. Research on spectral radius of graphs is nowadays very active, as seen from recent papers [4,13–15,17,18]. Easy verification shows that the Co-PI index of G can be expressed as one half of the sum of all entries of $M_{CPI}(G)$, i.e.,

$$Co - PI_v(G) = \frac{1}{2}\sum_{i=1}^{n} M_{CPI_i}(G)$$

where M_{CPI_i} is the sum of i-th row of the matrix M_{CPI}.

The notation of the energy of a graph was introduced by Ivan Gutman in [6] as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|$$

λ_i, $i = 1, ..., n$ are the eigenvalues of adjacency matrix of G. Details and more information on graph energy can be found in the recent books and papers [8–10, 16, 19, 22].

In a similar way, the Co-PI energy of a graph G,

$$Co - PIE(G) = \sum_{i=1}^{n} |\lambda_i^*|$$

is defined here.

In this paper, we give some bounds for the Co-PI spectral radius and the Co-PI energy for graphs.

2 Main Results

In this section, we give an upper bound for the Co-PI spectral radius and bounds on the second Co-PI spectral moment of a graph G. Also, we present an upper bound for the Co-PI energy of graphs and characterize those graphs for which this bound is the best possible.

Let $P(G; x) = x^n + c_1 x^{n-1} + ... + c_{n-1}x + c_n$ be the characteristic polynomial of G. N. Biggs proved that all coefficents of $P(G; x)$ can be expressed in terms of the principle minors of $\mathbf{A}(G)$, where a principle minor is the determinant of a submatrix obtained by taking a subset of the rows and that of columns. This leads to the following result.

Theorem 2.1. *[1] The coefficents of the characteristic polynomial $P(G;x)$ of a connected graph G satisfy: $c_1 = 0$, $-c_2$ is the number of edges and $-c_3$ is twice the number of triangles of G.*

Let $\mathbf{A}$ be the adjacency matrix of a graph G. It is well known that the $(i,j)-$th element $a_{ij}^{(k)}$ of the power matrix $\mathbf{A}^k$, $k \geq 1$, represents the number of walks of length k from the vertex u_i to the vertex u_j. Therefore, Su et al. deduced bounds on the second and third Co-PI spectral moment of a graph G.

Theorem 2.2. *[20] Let G be a connected graph with order $n \geq 3$, size m and t triangles. Then,*

$$\begin{aligned} 2m &\leq \lambda_1^{*^2} + \lambda_2^{*^2} + ... + \lambda_n^{*^2} \leq 2m(n-2)^2 \\ 6t &\leq \lambda_1^{*^3} + \lambda_2^{*^3} + ... + \lambda_n^{*^3} \leq 6t(n-2)^3. \end{aligned}$$

Now we use the relationship between the Co-PI index and Co-PI matrix to give bounds on the second Co-PI spectral moment of a graph in terms of its Co-PI index.

Theorem 2.3. *Let G be a graph with n vertices and m edges. Then,*

$$\begin{aligned} \frac{2}{m} Co-PI_v^2(G) &\leq \sum_{i=1}^{n} \lambda_i^{*^2} \leq \min\{2(n-2)Co-PI_v(G), \\ & \qquad 2m(n^2-2n+2) - 4Sz(G)\}. \end{aligned} \tag{1}$$

The left equaliy (1) holds if and only if $G \cong K_2$ and the right one if and only if $G \cong S_n$.

Proof. Let us denote $S = \sum_{i=1}^{n} \lambda_i^{*^2}$. It is enough to prove that $S \leq 2(n-2)Co-PI_v(G)$, $S \leq 2m(n^2-2n+2) - 4Sz(G)$. Obviously, $S = \left(\sum_{i=1}^{n} \lambda_i^*\right)^2 - 2\sum_{i<j} \lambda_i^* \lambda_j^* = -2\sum_{i<j} \lambda_i^* \lambda_j^*$ and $c_2 = \sum_{i<j} \lambda_i^* \lambda_j^*$. Therefore, $S = 2\sum_{i<j} \left(n_{v_j} - n_{v_i}\right)^2$ and since $\left|n_{v_j} - n_{v_i}\right| \leq (n-2)$, we have $S \leq 2(n-2)Co-PI_v(G)$.

On the other hand,

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

It is now easily seen that the equality is satisfied if and only if $\left|n_{v_i} - n_{v_j}\right| = (n-2)$, if and only if $n_{v_j} = n-1$ and $n_{v_i} = 1$, if and only if G is isomorphic to the star graph S_n.

The left inequality follows from the Cauchy-Schwarz inequality,

$$
\begin{aligned}
Co-PI_v(G) &= \sum_{e=v_iv_j} \left|n_{v_i} - n_{v_j}\right| \\
&\leq \sqrt{m\sum_{e=v_iv_j} \left|n_{v_i} - n_{v_j}\right|^2} = \sqrt{\frac{m}{2}S}.
\end{aligned}
$$

■

In the following theorem, we present an upper bound for λ_1^*.

Theorem 2.4. *Let G be a graph with n vertices and m edges. Then,*

$$
\lambda_1^* \leq \min\left\{ \begin{array}{c} \sqrt{\frac{2(n-1)(n-2)Co-PI_v(G)}{n}}, \\ \sqrt{\frac{(n-1)}{n}}\sqrt{2m(n^2-2n+2)-4Sz(G)} \end{array} \right\}. \tag{2}
$$

Proof. Since $\sum\limits_{i=1}^{n}\lambda_i^* = 0$, $\lambda_1^* = -\sum\limits_{i=2}^{n}\lambda_i^*$. Hence

$$
|\lambda_1^*| \leq \sum_{i=2}^{n}|\lambda_i^*| \leq \sqrt{n-1}\sqrt{\sum_{i=2}^{n}\lambda_i^{*^2}}.
$$

From there, we have

$$
\lambda_1^{*^2} \leq (n-1)\sum_{i=2}^{n}\lambda_i^{*^2} = (n-1)\left[\sum_{i=1}^{n}\lambda_i^{*^2} - \lambda_1^{*^2}\right].
$$

Therefore,

$$
\lambda_1^{*^2} \leq \frac{(n-1)}{n}\sum_{i=1}^{n}\lambda_i^{*^2}.
$$

The claim now follows by application of Theorem 2.3. ■

The first result of the Co-PI energy is the following.

Theorem 2.5. *Let G be a connected graph. Then,*

$$
Co-PIE(G) \leq \sqrt{2n\sum_{e=v_iv_j} \left|n_{v_i} - n_{v_j}\right|^2} \tag{3}
$$

Equality holds (3) if and only if G is empty. Moreover,

$$
Co-PIE(G) \leq \sqrt{n\alpha}
$$

in which

$$
\alpha = \min\left\{\sqrt{n}\sqrt{2(n-2)Co-PI_v(G)}, \sqrt{n}\sqrt{2m(n^2-2n+2)-4Sz(G)}\right\}.
$$

Proof. By definition of Co-PI energy and Theorem 2.3 we have,

$$Co-PIE(G)=\sum_{i=1}^{n}|\lambda_i^*|\leq\sqrt{n\sum_{i=1}^{n}\lambda_i^{*2}}=\sqrt{2n\sum_{e=v_iv_j}\left|n_{v_i}-n_{v_j}\right|^2}.$$

Therefore,

$$\begin{aligned}Co-PIE(G) &\leq \sqrt{n}\sqrt{2(n-2)Co-PI_v(G)}\\ Co-PIE(G) &\leq \sqrt{n}\sqrt{2m(n^2-2n+2)-4Sz(G)}\end{aligned}$$

which completes our theorem. ■

Let G be a graph with vertex set $V(G)=\{v_1,v_2,...,v_n\}$ and Co-PI matrix M_{CPI}. Then, the Co-PI degree of v_i, M_{CPI_i}, is given by $M_{CPI_i}=\sum_{j=1}^{n}c_{ij}$. Let $\{M_{CPI_1},M_{CPI_2},..,M_{CPI_n}\}$ be the Co-PI degree sequence. Then, the second Co-PI degree of v_i, denoted by MT_{CPI_i}, is given by $MT_{CPI_i}=\sum_{j=1}^{n}c_{ij}M_{CPI_j}$. If $\{M_{CPI_1},M_{CPI_2},..,M_{CPI_n}\}$ is the Co-PI degree sequence, then G is a k-Co-PI regular graph if $M_{CPI_i}=k$, for all i. If G has the Co-PI degree sequence and second Co-PI degree sequence $\{M_{CPI_1},M_{CPI_2},..,M_{CPI_n}\}$ and $\{MT_{CPI_1},MT_{CPI_2},...,MT_{CPI_n}\}$ respectively, then G is pseudo k-Co-PI regular graph if $\frac{MT_{CPI_i}}{M_{CPI_i}}=k$, for all i.

In order to obtain a different lower bound for the Co-PI energy of graphs, for each $i=1,2,...,n$, we define the sequence $C_i^{(1)},C_i^{(2)},...,C_i^{(t)},...$ as follows: For a fixed $\alpha\in\mathbb{R}$, let $C_i^{(1)}=M_{CPI_i}^{\alpha}$ and, for each $t\geq 2$, let $C_i^{(t)}=\sum_{i=1}^{n}c_{ij}C_j^{(t-1)}$.

The following Theorem is important for finding the upper bound for Co-PI energy.

Theorem 2.6. *[15] Let G be a connected graph, $\alpha\in\mathbb{R}$ and $t\in\mathbb{Z}$. Thus,*

$$\lambda_1^*\geq\sqrt{\frac{\sum_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum_{i=1}^{n}\left(C_i^{(t)}\right)^2}}\geq\sqrt{\frac{\sum_{i=1}^{n}(MT_{CPI_i})^2}{\sum_{i=1}^{n}(M_{CPI_i})^2}}.$$

Now, we have the following result.

Theorem 2.7. *Let G be a connected graph, $\alpha\in\mathbb{R}$ and $t\in\mathbb{Z}$. Thus,*

$$Co-PIE(G)\leq\sqrt{\frac{\sum_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum_{i=1}^{n}\left(C_i^{(t)}\right)^2}}+\sqrt{(n-1)\left[S-\frac{\sum_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum_{i=1}^{n}\left(C_i^{(t)}\right)^2}\right]}\qquad(4)$$

where S is the sum of the squares of entries in the Co-PI matrix. Equality holds in (4) if and only if G is a connected graph satisfying

$$\frac{C_1^{(t+1)}}{C_1^{(t)}} = \frac{C_2^{(t+1)}}{C_2^{(t)}} = ... = \frac{C_n^{(t+1)}}{C_n^{(t)}} = k \geq \sqrt{\frac{S}{n}}$$

with three distinct eigenvalues $\left(k, \sqrt{\frac{S-k^2}{n-1}}, -\sqrt{\frac{S-k^2}{n-1}}\right)$.

Proof. Let $\lambda_1^* \geq \lambda_2^* \geq ... \geq \lambda_n^*$ be the Co-PI eigenvalues of G.Then,

$$\sum_{i=1}^{n} \lambda_i^* = 0, \ \sum_{i=1}^{n} |\lambda_i^*| = Co - PIE(G)$$

and

$$\sum_{i=1}^{n} \lambda_i^{*^2} = S = \sum_{i,j=1}^{n} (c_{ij})^2.$$

By the Cauchy-Schwarz inequality we get,

$$\sum_{i=2}^{n} |\lambda_i^*| \leq \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i^{*^2}} = \sqrt{(n-1)(S - \lambda_1^{*^2})}. \tag{5}$$

Thus,

$$Co - PIE(G) \leq \lambda_1^* + \sqrt{(n-1)(S - \lambda_1^{*^2})}$$

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

$$M_{CPI_i}^2 = \left(\sum_{j=1}^{n} c_{ij}\right)^2 \leq n\sum_{j=1}^{n} c_{ij}^2$$

then,

$$\sum_{i=1}^{n} M_{CPI_i}^2 \leq \sum_{i=1}^{n} n \sum_{j=1}^{n} c_{ij}^2 = n\sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij}^2 = nS.$$

Also,

$$MT_{CPI_i} = \sum_{j=1}^{n} c_{ij} M_{CPI_j} \geq \sum_{j=1}^{n} c_{ij}^2$$

and

$$\sum_{i=1}^{n} MT_{CPI_i}^2 \geq \sum_{i=1}^{n} \left(\sum_{j=1}^{n} c_{ij}^2\right)^2 \geq S^2.$$

Hence by Theorem 2.6 , we have

$$\lambda_1^* \geq \sqrt{\frac{\sum\limits_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n}\left(C_i^{(t)}\right)^2}} \geq \sqrt{\frac{\sum\limits_{i=1}^{n}(MT_{CPI_i})^2}{\sum\limits_{i=1}^{n}(M_{CPI_i})^2}} \geq \sqrt{\frac{S^2}{nS}} = \sqrt{\frac{S}{n}}. \tag{6}$$

Therefore,

$$Co-PIE(G) \leq f(\lambda_1^*) \leq f\left(\sqrt{\frac{\sum\limits_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n}\left(C_i^{(t)}\right)^2}}\right)$$

and thus the theorem is proved. Now, we suppose the equality holds in (4). From (6) , we have

$$\lambda_1^* = \sqrt{\frac{\sum\limits_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n}\left(C_i^{(t)}\right)^2}}$$

which implies that

$$\frac{C_1^{(t+1)}}{C_1^{(t)}} = \frac{C_2^{(t+1)}}{C_2^{(t)}} = ... = \frac{C_n^{(t+1)}}{C_n^{(t)}}.$$

In particular, by (5), we find

$$|\lambda_i^*| = \sqrt{\frac{S-\lambda_1^{*2}}{n-1}}$$

for $i = 2, 3, ..., n$.Then, we have the following two possibilities:

- G has exactly one eigenvalue. Then all eigenvalues are zero as the sum of eigenvalues is the trace of M_{CPI} and as G is connected. So, $G \cong K_1$.
- G has exactly three distinct eigenvalues. In this case,

$$\lambda_1^* = \sqrt{\frac{\sum\limits_{i=1}^{n}\left(C_i^{(t+1)}\right)^2}{\sum\limits_{i=1}^{n}\left(C_i^{(t)}\right)^2}} \quad \text{and} \quad |\lambda_i^*| = \sqrt{\frac{S-\lambda_1^{*2}}{n-1}}$$

for $i = 2, 3, ..., n$. Since, $\frac{C_i^{(t+1)}}{C_i^{(t)}} = k$, for all i, we obtain that G is a connected graph with three distinct eigenvalues $\left(k, \sqrt{\frac{S-k^2}{n-1}}, -\sqrt{\frac{S-k^2}{n-1}}\right)$. Conversely, one can easily see that the equality in (4) holds for the graphs specified in the second part of the theorem. ■

For a special case, if we take $\alpha = 1$ and $t = 1$, we get the following result.

Corollary 2.8. *Let G be a graph with first and second Co-PI degree sequences*

$$\{M_{CPI_1}, M_{CPI_2}, .., M_{CPI_n}\} \text{ and } \{MT_{CPI_1}, MT_{CPI_2}, ..., MT_{CPI_n}\},$$

respectively. Then,

$$Co-PIE(G) \leq \sqrt{\frac{\sum\limits_{i=1}^{n}(MT_{CPI_i})^2}{\sum\limits_{i=1}^{n}(M_{CPI_i})^2}} + \sqrt{(n-1)\left[S - \frac{\sum\limits_{i=1}^{n}(MT_{CPI_i})^2}{\sum\limits_{i=1}^{n}(M_{CPI_i})^2}\right]}. \qquad (7)$$

where S is the sum of the squares of entries in the Co-PI matrix. Equality holds in (7) if and only if for a constant k, G is a pseudo k- Co-PI regular with three distinct eigenvalues $\left(k, \sqrt{\frac{S-k^2}{n-1}}, -\sqrt{\frac{S-k^2}{n-1}}\right)$.

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