On the Co-PI spectral radius and the Co-PI energy of graphs

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Motivation

This talk is based on the Co-PI spectral radius and the Co-PI energy of graphs. 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.

Motivation

A topological index is a number related to graph which is invariant under graph isomorphism. In theoretical chemistry, topological indices (also called molecular structure descriptors) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. By now there do exist a lot of different types of such indices which capture different aspects of the molecular graphs associated to the molecules considered.

Motivation

The Szeged index is closely related to *the Wiener index* and is a vertex-multiplicative type index that takes into account how the vertices of a given molecular graph are distributed. *The Padmakar-Ivan index* (*the PI index*) is an additive index that takes into account the distribution of edges.

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Here are the formulas of these topological indices:

$$PI_v(G) = \sum_{uv \in E(G)} n_u(e) + n_v(e) \qquad \textit{vertex PI index}$$

$$Sz(G) = \sum_{uv \in E(G)} n_u(e) n_v(e) \qquad \textit{Szeged index}$$

Some Fundamental Definitions

Now, we give some fundamental definitions which are used in our theorems. In this talk, G will denote a simple connected graph with n vertices and m edges without otherwise.

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Definition (2.1)

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.

Some Fundamental Definitions

Let $e = uv$ be an edge connecting vertices u and v in G.

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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.

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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

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

Some Fundamental Definitions

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

Hassani et al.-2010, Computation of the first vertex of Co-PI index of TUC4CS(S) nanotubes, *Iranian Journal of . Math. Chem.* 1 (1), (2010)119-123.

Some Fundamental Definitions

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.

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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: $w : E \rightarrow R^+ \cup \{0\}$ on E, which is said to be the *Co-PI weighting* of G.

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

Some Fundamental Definitions

Since Co-PI matrix is symmetric, all its eigenvalues $\lambda_i^*(G)$, $i = 1, 2, \cdots, n$, are real and can be labeled so that $\lambda_1^*(G) \geq \lambda_2^*(G) \geq \ldots \geq \lambda_n^*(G)$.

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

where $M_{CPI\,i}$ is the sum of *i-th row* of the matrix M_{CPI}.

Some Fundamental Definitions

The notation of the energy of a graph was introduced by Gutman-1978. It is defined as

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

λ_i, $i = 1, ..., n$ are the eigenvalues of adjacency matrix of G.

Gutman, The energy of a graph, Ber. Math. Stat. Sekt. Forschungsz. Graz 103, 1978, 1–22.

Some Fundamental Definitions

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

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

is defined here.

Preliminary Results

Fath-Tabar et al.-2010 proposed the Szeged matrix and Laplacian Szeged matrix. Then Su et al..-2013 introduced the Co-PI matrix of a graph.

Fath-Tabar et al.-2010, On the Szeged and the Laplacian Szeged spectrum of a graph, *Linear Algebra Appl.*, 433, (2010), 662-671.
Su et al.-2013, On the Co-PI and Laplacian Co-PI eigenvalues of a graph, *Discrete Applied Mathematics*,161 (2013) 277-283.

Preliminary Results

In the following, Su et al..-2013 characterised *the Co-PI spectra of Cartesian product graphs.*

Preliminary Results

Theorem (Su et al.-2013)

Let $G = G_1 \square G_2$ be the Cartesian product of two graphs G_1 and G_2. Then

$$\begin{aligned} \sigma'_{kl}\left(G_1 \square G_2\right) &= \left|V_1\right| \sigma'_l(G_2) + \left|V_2\right| \sigma'_k(G_1) \\ \text{for } k &= 1, 2, \ldots, \left|V_1\right| \text{ and } l = 1, 2, \ldots, \left|V_2\right|. \end{aligned}$$

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In here, σ' is the Co-PI eigenvalue and μ' is the Laplacian Co-PI eigenvalue of the graph.

Preliminary Results

Maden et al.-2011 found some bounds for the distance spectral radius and they characterized graphs for these bounds are attained. In another study, Maden et al.-2013 also presented some bounds for the resistance-distance spectral radius of a graph and one of these bounds depends on *the Kirchhoff index*.

Preliminary Results

Similarly, $\boxed{\text{Kaya et al..-2015}}$ found a lower bound for λ_1^* relating $Co - PI_v(G)$.

Preliminary Results

Corollary

Let G be a connected graph with $n \geq 2$. Then,

$$\lambda_1^* \geq \frac{2\left(Co - PI_v(G)\right)}{n}$$

with equality holding if and only if $M_{CPI_1} = M_{CPI_2} = \dots = M_{CPI_n}$.

Kaya et al.-2015, Bounds for the Co-PI Index of a Graph, *Iranian Journal of Mathematical Chemistry*, Vol. 6, No.1, 2015, 1-13.

Main Results

In this section, we give our results without proofs.

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Let $P(G;x) = x^n + c_1x^{n-1} + ... + c_{n-1}x + c_n$ 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 $A(G)$, 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.

Main Results

Theorem (Biggs)

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.

Main Results

Theorem (Su et al..-2013)

Let G be a connected graph with order $n \geq 3$, size m and t triangles. Then

$$2m \leq \sigma_1'^2 + \sigma_2'^2 + ... + \sigma_n'^2 \leq 2m(n-2)^2.$$

$$6t \leq \sigma_1'^3 + \sigma_2'^3 + ... + \sigma_n'^3 \leq 6t(n-2)^3.$$

The first result of this paper is the following.

Main Results

Theorem

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

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

The left equaliy holds if and only if G is complete bipartite graph and the right one if and only if G is star graph.

Main Results

The next is another result.

Lemma

Let G be a graph on n vertices and λ^* any of its Co-PI eigenvalues. Then

$$|\lambda^*| \leq (n-2)\Delta(G),$$

where $\Delta(G)$ denotes the largest degree of a vertex in G.

Main Results

Theorem

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

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

Main Results

Theorem

Let G be a connected graph. Then,

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

Equality holds if and only if G is empty.

Main Results

Theorem

Moreover,

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

in which

$$\begin{aligned}\alpha &= \min\{\sqrt{n}\sqrt{2(n-2)Co-PI_v(G)}, \\ &\sqrt{n}\sqrt{2m(n^2-2n+2)-4Sz(G)} \\ &, \sqrt{n}\sqrt{2Co-PI_v(G)^2-2m(m-1)}\}\end{aligned}$$

Main Results

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 $C_i^{(t)} = \sum_{i=1}^{n} cijC_j^{(t-1)}$. We then have the following result.

Theorem

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

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

For particular values of α and t, the above equality holds if and only if

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

Main Results

Theorem

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

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

where S is the sum of the squares of entries in the Co-PI matrix.

Main Results

Theorem

Equality holds if and only if G is a connected graph satisfying

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

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

Main Results

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

Theorem

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,

$$Co-PIE(G) \leq \sqrt{\frac{\sum_{i=1}^{n}(MT_{CPI_i})^2}{\sum_{i=1}^{n}(M_{CPI_i})^2}} + (n-1)\sqrt{S - \frac{\sum_{i=1}^{n}(MT_{CPI_i})^2}{\sum_{i=1}^{n}(M_{CPI_i})^2}}.$$

Main Results

Theorem

where S is the sum of the squares of entries in the Co-PI matrix. Equality holds 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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