Motivation

Some Fundamental Definitions

Preliminary Results

Main Results

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

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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.
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.
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. Here are the formulas of these topological indices:
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Here are the formulas of these topological indices:

\[
PI_v(G) = \sum_{uv \in E(G)} n_u(e) + n_v(e) \quad \text{vertex PI index}
\]

\[
Sz(G) = \sum_{uv \in E(G)} n_u(e)n_v(e) \quad \text{Szeged index}
\]
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 \( G \).
Let $e = uv$ be an edge connecting vertices $u$ and $v$ in $G$. Define the sets:

$$N_u(e) = \{z \in V \mid d_G(z, u) < d_G(z, v)\}$$
$$N_v(e) = \{z \in V \mid d_G(z, v) < d_G(z, u)\}$$

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

$$n_u(e) = |N_u(e)| \quad \text{and} \quad n_v(e) = |N_v(e)|.$$
Hassani et al.-2010 introduced the following vertex Co-PI index and computed this index for $TUC_4C_8(R)$ nanotubes.
Hassani et al.-2010 introduced the following vertex Co-PI index and computed this index for $TUC_4 C_8(R)$ nanotubes.

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

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 \( j \).
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 $j$. 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 $G$. 
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 $G$. 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,

$$c_{ij} = \begin{cases} |n_{v_i}(e) - n_{v_j}(e)|, & e = v_i v_j \\ 0, & otherwise \end{cases}.$$
Since Co-PI matrix is symmetric, all its eigenvalues $\lambda_i^*(G)$, $i = 1, 2, \ldots, n$, are real and can be labeled so that $\lambda_1^*(G) \geq \lambda_2^*(G) \geq \ldots \geq \lambda_n^*(G)$. 
Some Fundamental Definitions

Since Co-PI matrix is symmetric, all its eigenvalues $\lambda_i^*(G)$, $i = 1, 2, \ldots, n$, are real and can be labeled so that $\lambda_1^*(G) \geq \lambda_2^*(G) \geq \ldots \geq \lambda_n^*(G)$. 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 $Co-PI-Spec(G)$. 
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 $\lambda_1^*(G) \geq \lambda_2^*(G) \geq \cdots \geq \lambda_n^*(G)$. The eigenvalues of $M_{CPI}$ are said to be \textit{the Co-PI eigenvalues} of $G$ and the $M_{CPI}$–spectrum of $G$ is denoted by $\text{Co-PI-Spec}(G)$. 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.,

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

where $M_{CPI_i}$ is the sum of \textit{i-th row} of the matrix $M_{CPI}$.
The notation of the energy of a graph was introduced by Gutman-1978. It is defined as

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

\(\lambda_i, \ i = 1, ..., n\) are the eigenvalues of adjacency matrix of \(G\).

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

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

is defined here.
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.

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

\[
\sigma'_{kl} (G_1 \square G_2) = |V_1| \sigma'_l (G_2) + |V_2| \sigma'_k (G_1)
\]

for \( k = 1, 2, \ldots, |V_1| \) and \( l = 1, 2, \ldots, |V_2| \).

\[
\mu'_{kl} (G_1 \square G_2) = |V_1| \mu'_l (G_2) + |V_2| \mu'_k (G_1)
\]

for \( k = 1, 2, \ldots, |V_1| \) and \( l = 1, 2, \ldots, |V_2| \).

In here, \( \sigma' \) is the Co-PI eigenvalue and \( \mu' \) is the Laplacian Co-PI eigenvalue of the graph.
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.
Similarly, Kaya et al. - 2015 found a lower bound for $\lambda_1^*$ relating $Co - PL_v(G)$. 
Corollary

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

$$\lambda_1^* \geq \frac{2 (\text{Co-PI}_v(G))}{n}$$

with equality holding if and only if $M_{\text{CPI}_1} = M_{\text{CPI}_2} = \ldots = M_{\text{CPI}_n}$.

In this section, we give our results without proofs.
In this section, we give our results without proofs. Let $P(G; x) = x^n + c_1x^{n-1} + \ldots + c_{n-1}x + c_n$ be the characteristic polynomial of $G$. N. Biggs proved that all coefficients 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.
Theorem (Biggs)

The coefficients 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

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

$$6t \leq \sigma_1^3 + \sigma_2^3 + \ldots + \sigma_n^3 \leq 6t(n - 2)^3.$$  

The first result of this paper is the following.
Theorem

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

\[
\frac{2}{m} \text{Co} - \text{PI}_v^2(G) \leq \lambda_i^2 \leq \min\{2(n - 2)\text{Co} - \text{PI}_v(G),
2m(n^2 - 2n + 2) - 4\text{Sz}(G),
2\text{Co} - \text{PI}_v^2(G) - 2m(m - 1)\}.
\]

The left equality holds if and only if \( G \) is complete bipartite graph and the right one if and only if \( G \) is star graph.
The next is another result.

**Lemma**

Let $G$ be a graph on $n$ vertices and $\lambda^*$ 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,

$$\lambda_1^* \leq \min \left\{ \sqrt{\frac{2(n-1)(n-2)\text{Co-PI}_v(G)}{n}}, \sqrt{\frac{2m(n^2-2n+2)-4\text{Sz}(G)(n-1)}{n}}, \sqrt{\frac{n-1}{n}} \sqrt{2\text{Co} - \text{PI}_v(G)^2 - 2m(m-1)} \right\} $$
Theorem

Let $G$ be a connected graph. Then,

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

Equality holds if and only if $G$ is empty.
Main Results

Theorem

Moreover,

\[ \text{Co} - \text{PIE}(G) \leq \sqrt{n\alpha} \]

in which

\[ \alpha = \min\{ \sqrt{n}\sqrt{2(n-2)\text{Co} - \text{Pl}_v(G)}, \sqrt{n}\sqrt{2m(n^2 - 2n + 2) - 4Sz(G)} \}, \sqrt{n}\sqrt{2\text{Co} - \text{Pl}_v(G)^2 - 2m(m - 1)} \} \]
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 $C_i^{(1)} = M_{CPI}^\alpha$, and, for each $t \geq 2$, let $C_i^{(t)} = \sum_{j=1}^{n} c_{ij} C_j^{(t-1)}$. 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 $\alpha$ 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,

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

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

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

$$\{M_{CPI_1}, M_{CPI_2}, \ldots, M_{CPI_n}\} \quad \text{and} \quad \{M_{T_{CPI_1}}, M_{T_{CPI_2}}, \ldots, M_{T_{CPI_n}}\},$$

respectively. Then,

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

$$
\left( k, \sqrt{\frac{S-k^2}{n-1}}, -\sqrt{\frac{S-k^2}{n-1}} \right).
$$
THANK YOU FOR YOUR ATTENTION...


A. D. Maden (Güngör), Ş. B. Bozkurt, On the Distance Spectral Radius and the Distance Energy of Graphs, Linear and Multilinear Algebra, 29 (4), 2011, 365-370.


