Some results on the smallest positive eigenvalue of trees

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Introduction

A graph is an ordered pair $G = (V(G), E(G))$, where $V(G)$ is set of vertices of G, and $E(G)$ is set of edges of G.

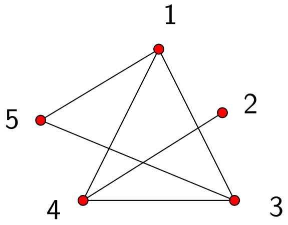
We shall consider simple graphs only.

Adjacency matrix $A(G) = [a_{ij}]$ is defined as

$$a_{ij} = \begin{cases} 1 & \text{if } i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Example

Consider the following graph:



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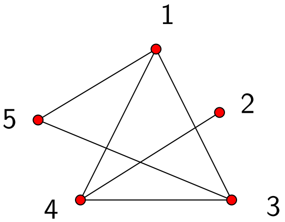

$$A(G) = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

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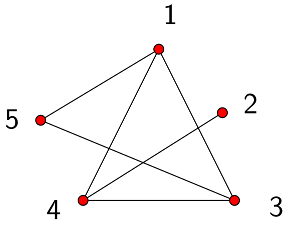

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$$\sigma(G) = \{2.64, 0.72, -0.59, -1, -1.78\}$$

The largest eigenvalue (spectral radius) of $G = \rho(G)$

The smallest positive eigenvalue of $G = \tau(G)$

Spectrum and structural properties of a graph

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of a graph G. Then

- G is bipartite if and only if $\lambda_1 = -\lambda_n$.
- G is complete if and only if $\lambda_2 = -1$.
- $\lambda_3 = -1$ if and only if G^c is isomorphic to the union of a complete bipartite graph and some isolated vertices.
- $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 2|E(G)|$.
- $\lambda_1^3 + \lambda_2^3 + \cdots + \lambda_n^3 = 6|T(G)|$, where $T(G)$ is number of triangles in G.

Spectral Graph Theory

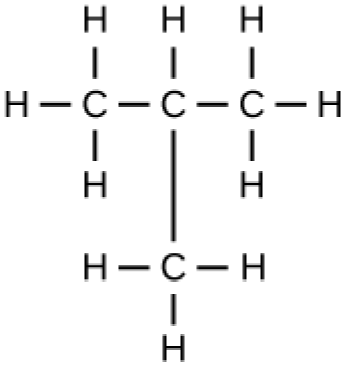
Some of the popular research problems are

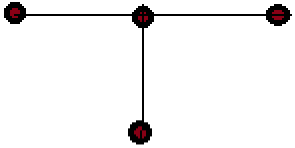
1. To find bounds on a particular eigenvalue
2. To compare an eigenvalue in two different graphs
3. To find a graph having the maximum or the minimum value of an eigenvalue in a class of graphs
4. To find a pair of non co-spectral graphs which share a particular eigenvalue
5. To find a relation between an eigenvalue and other graph parameters

We consider the smallest positive eigenvalue.

Hückel Graph

Graph representation of a molecule





An isobutane molecule and its Hückel graph

Graph theory terms in chemistry

Graph	Conjugated Hydrocarbon
Vertex	Carbon atom
Edge	Carbon-carbon bond
Adjacency matrix	Huckel Matrix, topological matrix
Bipartite graph	Alternant hydrocarbon

Alternant hydrocarbons are the molecules of immense interest in mathematical chemistry.

Various energies in terms of graph spectra

For alternant hydrocarbons possessing $2n$ conjugated carbon atoms,

- The total π-electron energy is $2\sum_{i=1}^{n}\lambda_i$,
- The HOMO energy is λ_n,
- The LUMO energy is $-\lambda_n$,
- The HOMO LUMO sepeartion is $2\lambda_n$.

HOMO: Highest Occupied Molecular Orbit

LUMO: Lowest Unoccupied Molecular Orbit

λ_n: The smallest positive eigenvalue of adjacency matrix

Larger the HOMO LUMO separation, more reactive is underlying π-electron system.

The variation in λ_n from a molecule to molecule follows too complicated a pattern to be summarized in general rules.

- G.G.Hall (1977)

Important results from literature

Gutman conjectured among all non-singular trees on n vertices, P_n, the path graph on n vertices has the minimum smallest positive eigenvalue.

Godsil (1985) proved the conjecture true.

Theorem (Hong, 1989)

For any tree T on n vertices, $\tau(T) \geq \tau(P_n)$ and equality occurs if and only if $T = P_n$.

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Theorem (Pavlíková and Krc-Jediný 1990, Shao and Hong 1992)

Among all non-singular trees on n vertices, the comb graph alone has the maximum smallest positive eigenvalue.

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- Chen and Zhang (2018) provided an upper bound on the smallest positive eigenvalue of non-singular trees with maximum degree at most 3 and order greater than 11.
- Rani and Barik (2020) determined the tree on n vertices with the second, third and the fourth minimum smallest positive eigenvalue.

Terminology

- A tree is connected acyclic graph.
- A tree is non-singular if its adjacency matrix is non-singular.
- A pendant is a vertex of degree 1.
- A quasipendant is the vertex adjacent to a pendant.
- $N(u) = \{v : v \sim u\}$ is the set of neighbors of u.
- $\widehat{G}(v)$ is the graph obtained from G by attaching a pendant at vertex v of G.

Perturbation by attaching a pendant

Theorem

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Let $n \geq 4$ and G be a graph on n vertices with a quasipendant vertex v. Then $\tau(G) \leq \tau(\widehat{G}(v))$.

Attaching a pendant in a non-singular tree

Theorem

For a non-singular tree T, $\tau(T) \leq \tau(\widehat{T}(v))$ for every $v \in V(T)$.

Outline of proof: Attaching a pendant does not change the number of nonzero eigenvalues in T but it increases the order by 1. Now by Cauchy Interlacing Theorem, the result follows.

An immediate question

- Does there exist a singular tree such that $\tau(T) > \tau(\widehat{T}(v))$ for every $v \in V(T)$?

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NO.

We prove the result by showing that if u and v are adjacent in a tree and $\tau(T) > \tau(\widehat{T}(u))$ then $\tau(T) \leq \tau(\widehat{T}(v))$.

Two important results

Theorem 1

Let T be a tree on vertices $1, 2, \ldots, n$ and R_i be the row indexed by vertex i in $A(T)$ for $i = 1, 2, \ldots, n$. If $\tau(T) > \tau(\widehat{T}(i))$ Then $R_i \in \text{Span}\{R_1, R_2, \ldots, R_{i-1}, R_{i+1}, \ldots, R_n\}$.

Proof is by contradiction. Let $R_i \notin \text{Span}\{R_1, R_2, \ldots, R_{i-1}, R_{i+1}, \ldots, R_n\}$ then it is a linearly independent row. Adding a pendant at i can not make it dependent. So, T and $\widehat{T}(i)$ have same rank and then interlacing of eigenvalues of T and $\widehat{T}(i)$ produce a contradiction to $\tau(T) > \tau(\widehat{T}(i))$.

Results continued...

Theorem 2

Let T be a tree on vertices $1, 2, \ldots, n$ and R_i be the row indexed by vertex i in $A(T)$ for $i = 1, 2, \ldots, n$. If u, v are two adjacent vertices of T and $R_u \in \text{Span}\{R_1, R_2, \ldots, R_{u-1}, R_{u+1}, \ldots, R_n\}$. Then $R_v \notin \text{Span}\{R_1, R_2, \ldots, R_{v-1}, R_{v+1}, \ldots, R_n\}$.

An example

$$A(P_5) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

$R_5 = R_3 - R_1$ but R_4 can not be written as linear combination of other rows of $A(P_5)$.

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Theorem 3

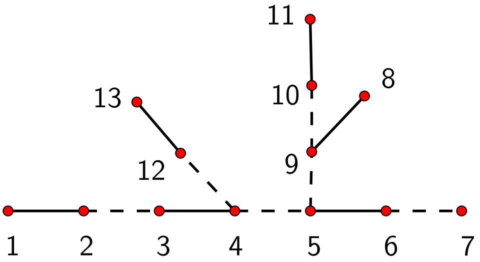
Let T be a tree and $[u, v]$ be an edge in T such that $\tau(\widehat{T}(u)) < \tau(T)$. Then $\tau(\widehat{T}(v)) \geq \tau(T)$.

A natural question

- Can we provide a characterization of vertices u and v in a tree T such that $\tau(\widehat{T}(u)) \leq \tau(T)$ and $\tau(\widehat{T}(v)) \geq \tau(T)$?

Matching

Matching of a graph G is a collection of edges in G such that no two of the edges share a common vertex. Edges lying inside matching are matching edges and others are non-matching edges. Vertex lying on the matching edges are known to be saturated by that matching.



Matching

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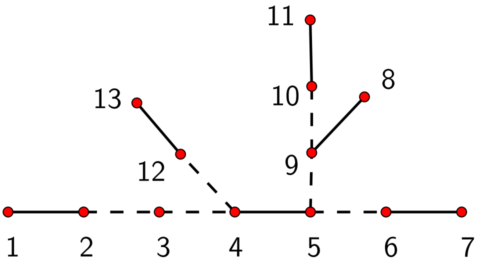


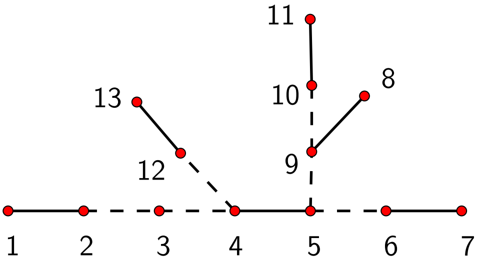
Characterization of vertices in a singular tree

Theorem

Let T be a tree and $\mathcal{M}(T)$ be a maximum matching of T. Let U be the set of vertices which are unsaturated by $\mathcal{M}(T)$. Let $\mathcal{F}_1 = U$ and
$\mathcal{F}_i = \{v : [v, u] \in \mathcal{M}(T), u \in N(w)$ for some $w \in \mathcal{F}_{i-1}\}$ for $i \geq 2$. Let $\mathcal{F} = \cup \mathcal{F}_i$. Then

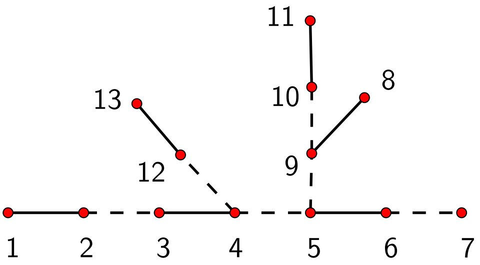
1. $\tau(T) \geq \tau(\widehat{T}(i))$ for each $i \in \mathcal{F}$,
2. $\tau(T) \leq \tau(\widehat{T}(i))$ for each $i \in V(T) \setminus \mathcal{F}$.

Example



Vertex 3 is unsaturated, so, $\mathcal{F}_1 = \{3\}$. Now $N(3) = \{4, 2\}$ so, $\mathcal{F}_2 = \{5, 1\}$. $N(5) = \{4, 6, 9\}$ and $N(1) = \{2\}$. So, $\mathcal{F}_3 = \{7, 8\}$. Again $7, 8$ themselves are matching mates of their neighbors. Thus, $\mathcal{F} = \{3, 5, 1, 7, 8\}$. By Matlab calculation, we see that $\tau(T) = 0.5140$, $\tau(\widehat{T}(3)) = 0.3001, \tau(\widehat{T}(5)) = 0.3478, \tau(\widehat{T}(1)) = 0.2621, \tau(\widehat{T}(7)) = 0.2928, \tau(\widehat{T}(8)) = 0.2542$, $\tau(\widehat{T}(2)) = 0.5608, \tau(\widehat{T}(4)) = 0.6473, \tau(\widehat{T}(6)) = 0.5222, \tau(\widehat{T}(9)) = 0.5262, \tau(\widehat{T}(10)) = 0.5436, \tau(\widehat{T}(11)) = 0.5737, \tau(\widehat{T}(12)) = 0.6523, \tau(\widehat{T}(13)) = 0.5463,$.

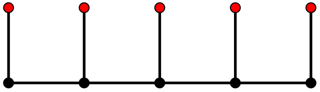
Example



Vertex 7 is unsaturated, so, $\mathcal{F}_1 = \{7\}$. Now $N(7) = \{6\}$ so, $\mathcal{F}_2 = \{5\}$. $N(5) = \{4, 6, 9\}$. So, $\mathcal{F}_3 = \{3, 8\}$. Again $N(3) = \{4, 2\}$ and $N(8) = \{9\}$. So $\mathcal{F}_4 = \{1\}$.Thus, $\mathcal{F} = \{7, 5, 3, 8, 1\}$.

Corona tree

- Corona tree of a tree T is obtained by attaching a pendant vertex at each vertex of T, and is denoted by $\tilde{T}$.
- If λ is an eigenvalue of T, then $\frac{\lambda \pm \sqrt{\lambda^2+4}}{2}$ are the eigenvalues of $\tilde{T}$.
- $\rho(\tilde{T}) = \frac{\rho(T)+\sqrt{\rho(T)^2+4}}{2}$
- $\tau(\tilde{T}) = \frac{\rho(T)-\sqrt{\rho(T)^2+4}}{2}$



$\tilde{P}_5$

A graph operation

Definition (Xu 1997)

Let T be a tree and $[u, v]$ be an edge in T such that each of the vertices u and v has degree at least two. Denote by $T[u, v]$, the tree obtained from T by deleting the edge $[u, v]$, identifying the vertices u and v (suppose that the new vertex is still denoted by u), and then attaching a new pendant vertex v at u.

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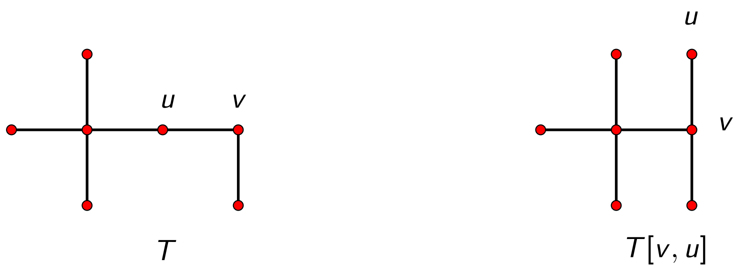

A helpful Lemma

A matching which saturates every vertex is known as perfect matching.

Lemma (Barik, Neumann and Pati 2006)

Let T be a non-singular tree with a perfect matching $\mathcal{M}$. If T is not a corona tree, then T has two vertices i and j of degree at least two such that $[i, j] \in \mathcal{M}$ and $\tau(T[i, j]) > \tau(T)$.

The maximal non-singular tree on n vertices

Theorem

For every non-singular non-corona tree T on n vertices, there exist a corona tree T' on n vertices such that $\tau(T) < \tau(T')$.

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Corollary

Let T be a non-singular tree on $2n$ vertices. Then

$$\tau(T) \leq \sqrt{cos^2(\pi/(n+1)) + 1} - cos(\pi/(n+1))$$

and equality holds if and only if $T = \tilde{P}_n$.

A construction of graphs having the same $\tau(T)$

Construction

If n is even, then there exist vertices i and j in P_{2n} such that $\tau(\widehat{P}_{2n}(i)) = \tau(\widehat{P}_{2n}(j))$.

Theorem

For $k \geq 1$, $\tau(\widehat{P}_{4k}(2k-1)) = \tau(\widehat{P}_{4k}(1))$.

Construction

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Example: If we take $k = 2$, then the two trees are $\widehat{P}_8(3)$ and $\widehat{P}_8(1)$ and the smallest positive eigenvalue for both the trees is 0.6180.

Construction

If n is odd, there may not exist two vertices i and j in P_{2n} such that $\tau(\widehat{P}_{2n}(i)) = \tau(\widehat{P}_{2n}(j))$.

Example

Consider $n = 5$, take P_{10} and obtain $\widehat{P}_{10}(i)$ for $i = 1, 2, \ldots, 5$. Matlab computation of $\tau(\hat{P}_{10}(i))$ gives
$\tau(\widehat{P}_{10}(1)) = 0.5176, \tau(\widehat{P}_{10}(2)) = 0.3129, \tau(\widehat{P}_{10}(3)) = 0.5509, \tau(\widehat{P}_{10}(4)) = 0.3731$ and $\tau(\widehat{P}_{10}(5)) = 0.4648$.

Here no two graphs have the same smallest positive eigenvalue.

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Thank you!