

Median Eigenvalues and Graph Inverse

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Let G be a graph with edge set $E(G)$ and vertex set $V(G)$. The **adjacency matrix** of G is defined as

$$\mathbb{A} = [a_{ij}]$$

where $a_{ij} = 1$ if $ij \in E(G)$ and $a_{ij} = 0$ otherwise.

Graphs and Matrices

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where $a_{ij} = 1$ if $ij \in E(G)$ and $a_{ij} = 0$ otherwise.

The **eigenvalues of \mathbb{A}** are also called the **eigenvalues of the graph G** , denoted by $\lambda_1(G) \geq \dots \geq \lambda_n(G)$.

Median Eigenvalues

Two **median eigenvalues** are denoted by $\lambda_H(G)$ and $\lambda_L(G)$, where $H = \lfloor \frac{n+1}{2} \rfloor$ and $L = \lceil \frac{n+1}{2} \rceil$.

Median Eigenvalues

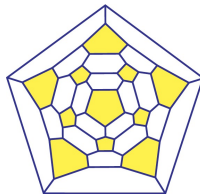
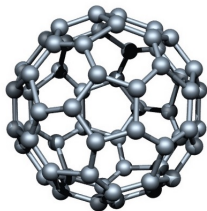
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- HOMO-LUMO gap: $\Delta = \lambda_H - \lambda_L$.

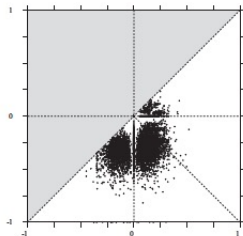
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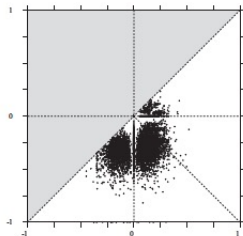


Median Eigenvalues



HOMO-LUMO map for the 7595 20-vertex cubic polyhedra.

Median Eigenvalues



HOMO-LUMO map for the 7595 20-vertex cubic polyhedra.

- **CONJECTURE (FOWLER & PISANSKI, 2010)** There are **finitely many** subcubic graphs with $\lambda_H, \lambda_L \notin [-1, 1]$.

Bounding Median Eigenvalues: Graph Partition

- **Interlacing Theorem:** Let \mathbb{A} be an $n \times n$ symmetric matrix with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let B be an $(n - k) \times (n - k)$ symmetric minor of \mathbb{A} with eigenvalues $\mu_1 \geq \cdots \geq \mu_{n-k}$. Then $\lambda_i \leq \mu_i \leq \lambda_{i+k}$.

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- **Graph Partition:** A partition $\{V_1, V_2\}$ of $V(G)$ is **unfriendly** if every vertex in V_1 has at least as many neighbors in V_2 as in V_1 . A partition is **unbalanced** if $|V_1| \neq |V_2|$.

Bounding Median Eigenvalues: Graph Partition

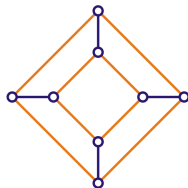
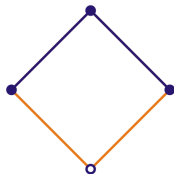
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- CONJECTURE (MOHAR, 2012) Every plane subcubic graph has $\lambda_H, \lambda_L \in [-1, 1]$.

Bounding Median Eigenvalues: Graph Partition

- (Y., 2017+) Let G be a 2-connected plane cubic graph different from K_4 . Then G has an unfriendly unbalanced partition if and only if G has no 4-cycle 2-factor.

Bounding Median Eigenvalues: Graph Partition

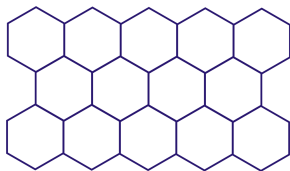
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- (Y., 2017+) Let G be a 2-connected plane cubic graph without a 4-cycle 2-factor. Then $\lambda_H(G), \lambda_L(G) \in [-1, 1]$.

Bounding Median Eigenvalues: Graph Square

- The **square** of a graph G is another graph with the same vertex set as G and two vertices are adjacent if they have distance two in G , denoted by G^2 .

Bounding Median Eigenvalues: Graph Square

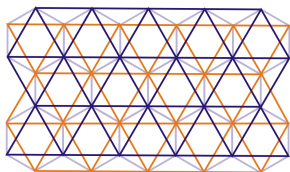
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Adjacency matrix A

Bounding Median Eigenvalues: Graph Square

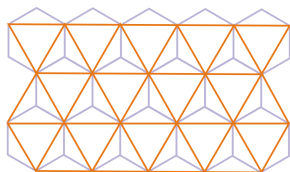
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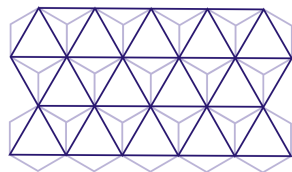
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Adjacency matrix B_*



Adjacency matrix B_o

Bounding Median Eigenvalues: Graph Square

Let G be a bipartite graph with adjacency matrix $A = \begin{bmatrix} 0 & B \\ B^\top & 0 \end{bmatrix}$. Denote $B_* = BB^\top$ and $B_o = B^\top B$.

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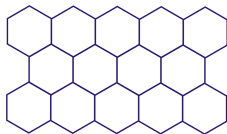
- $A^2 = \begin{bmatrix} B_* & 0 \\ 0 & B_o \end{bmatrix}$
- $\max\{|\lambda_L|, |\lambda_H|\} \leq \min\{\sqrt{\lambda_{\min}(B_*)}, \sqrt{\lambda_{\min}(B_o)}\}$

Bounding Median Eigenvalues: Graph Square

A **hexagonal system** (graphene) is a bipartite plane graph with only hexagon as inner faces.

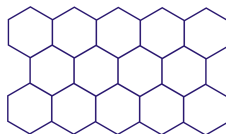
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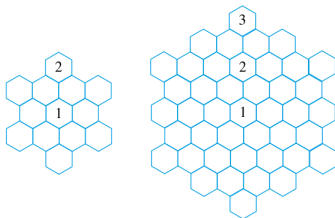


- (KLEIN, YANG AND Y., 2015) A hexagonal system has median eigenvalues

$$-\sqrt{\frac{n_2}{n}} \leq \lambda_L \leq \lambda_H \leq \sqrt{\frac{n_2}{n}}.$$

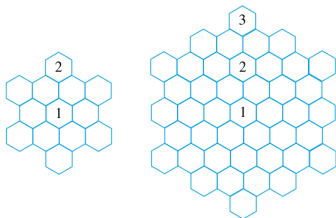
Bounding Median Eigenvalues: Graph Square

- Ring-type hexagonal systems: $\Delta \leq \sqrt{(8x - 4)/(3x^2 - 3x + 1)}$ where x is the number of rings.



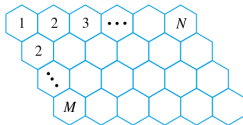
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- Parallelogram-like hexagonal systems:

$$\Delta \leq 2\sqrt{(M + N + 1)/(MN + M + N)}.$$



Bounding Median Eigenvalues: Graph Inverse

- Rayleigh-Quotient method:

$$\lambda_1(G) = \max_{\mathbf{x} \in \mathbb{R}^n} \frac{\langle \mathbf{x}, \mathbf{A}\mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle};$$

$$\lambda_n(G) = \min_{\mathbf{x} \in \mathbb{R}^n} \frac{\langle \mathbf{x}, \mathbf{A}\mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle}.$$

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- The spectrum of a graph G is **symmetric** about the origin if and only if G is bipartite graph.

If \mathbb{A} is invertible, then $\lambda_H(G) = 1/\lambda_1(\mathbb{A}^{-1})$ and $\lambda_L(G) = 1/\lambda_n(\mathbb{A}^{-1})$.

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- For non-bipartite graph, the method works as long as the spectrum **splits** about the origin (i.e., half number of eigenvalues are positive and half of them are negative), such as leapfrog fullerenes.

Graph Inverse

- (HARARY, 1962) Let G be a connected graph and \mathbb{A} , the adjacency matrix of G . Then \mathbb{A} is invertible and its inverse is an adjacency matrix of a graph if and only if G is K_2 .

Graph Inverse

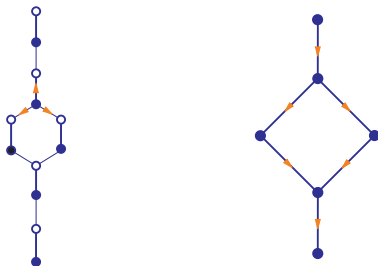
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- (GODSIL, 1986) Define inverse for bipartite graphs G with unique perfect matching.

A bipartite graph G is *invertible* if \mathbb{A} is invertible and diagonally similar to a non-negative matrix (i.e. there exists a diagonal matrix \mathbb{D} with entry in $\{0, 1, -1\}$ such that $\mathbb{D}\mathbb{A}^{-1}\mathbb{D}$ is an adjacency matrix of a graph).

Graph Inverse

- (SIMON & CAO, 1989) Let G be a bipartite graph with a bipartition (R, C) . Let D be the digraph obtained from G by orienting edges from R to C and then contracting all edges in M . Then D is acyclic.



Graph Inverse

- For the digraph D , define a poset (\mathcal{P}, \leq) such that $\mathcal{P} = V(D)$ and $a_i \leq a_j$ if and only if there is a directed path from a_i to a_j ,

$$(\mathbb{M}(x))_{ij} := \begin{cases} 1 & \text{if } a_i a_j \text{ is an arc of } D; \\ x & \text{if } a_i a_j \notin E(D) \text{ and } a_i \leq a_j \text{ in } \mathcal{P}; \\ 0 & \text{otherwise.} \end{cases}$$

- $\mathbb{M}(1)$ is the Zeta-function matrix of \mathcal{P} and $\mathbb{M}(0) = \mathbb{B}$ is the adjacency matrix of D .
- (Lovász, 1979) $\mathbb{M}^{-1}(1)$ is the Möbius-function matrix of \mathcal{P} and $\mathbb{M}^{-1}(0)$ is the inverse of bipartite adjacency matrix of G .

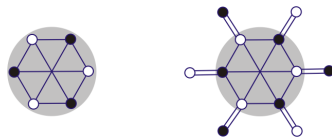
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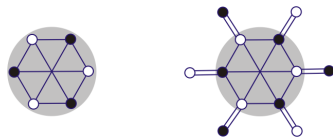
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- (AKBARI & KIRKLAND, 2007) Characterize all invertible unicycle graphs.

- **DEFINITION.** Let (G, ω) be a weighted graph with $\omega : E(G) \rightarrow \mathbb{F} \setminus \{0\}$ where \mathbb{F} is a feild. Let \mathbb{A} be the adjacency matrix of (G, ω) defined by $\mathbb{A}_{i,j} = \omega(ij)$ if $ij \in E(G)$ and 0 otherwise.

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- If \mathbb{A} is invertible, then its inverse is **symmetric** and hence is an adjacency matrix of a weighted graph, denoted by (G^{-1}, ω^{-1}) .

Graph Inverse

A spanning subgraph S is a **2-matching** if every component of G is either K_2 or a cycle (including loop). Let $S = \mathcal{C} \cup M \cup L$ where $\mathcal{C} = \{\text{all cycles of } S\}$, $L = \{\text{all loops of } S\}$ and $M = \{\text{all } K_2 \text{ of } S\}$.

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A spanning subgraph S is a **2-matching** if every component of G is either K_2 or a cycle (including loop). Let $S = C \cup M \cup L$ where $C = \{\text{all cycles of } S\}$, $L = \{\text{all loops of } S\}$ and $M = \{\text{all } K_2 \text{ of } S\}$.

- (**HARARY 1967**) Let (G, ω) be a weighted graph and \mathbb{A} the adjacency matrix. Then

$$\det(\mathbb{A}) = \sum_S 2^{|\mathcal{C}|} \omega(\mathcal{C} \cup L) \omega^2(M) (-1)^{|\mathcal{C}| + |L| + |E(S)|},$$

where $S = C \cup M \cup L$ is a 2-matching.

Graph Inverse

- (KLEIN, MANDEL, YANG & Y., 2017) Let (G, ω) be a weighted graph with adjacency matrix \mathbb{A} , and

$$\mathcal{P}_{ij} = \{P \mid P \text{ joins } i \text{ and } j \text{ such that } G - V(P) \text{ has a 2-matching } S\}.$$

If (G, ω) has an inverse (G^{-1}, ω^{-1}) , then

$$\omega^{-1}(ij) = \frac{1}{\det(\mathbb{A})} \sum_{P \in \mathcal{P}_{ij}} \left(\omega(P) \left(\sum_S \omega(\mathcal{C} \cup L) \omega^2(M) 2^{|\mathcal{C}|} (-1)^{|\mathcal{C}|+|L|+|E(S) \cup E(P)|} \right) \right)$$

where $S = \mathcal{C} \cup M \cup L$ is a 2-matching of $G - V(P)$.

Graph Inverse

- Let G be a bipartite graph with a unique perfect matching M . Then G has an inverse (G^{-1}, w^{-1}) such that

$$w^{-1}(ij) = \begin{cases} \sum_P (-1)^{|E(P) \setminus M|} & \text{if } i \neq j; \\ 0 & \text{if } i = j. \end{cases}$$

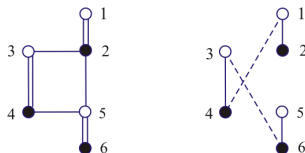
where P is an M -alternating path of G .

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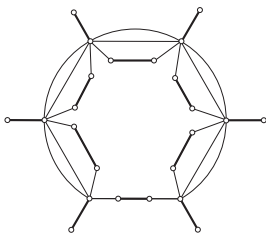
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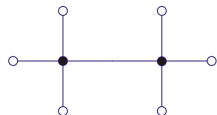


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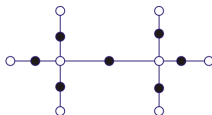
- (YANG & Y., 2015+) Let G be a bipartite graph with a unique perfect matching M . Then \mathbb{A}^{-1} is diagonally similar to a non-negative matrix if and only if G does not contain an odd flower.



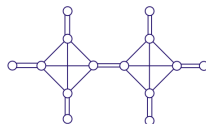
Bounding Median Eigenvalues



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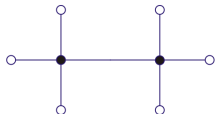
$\text{sub}(T)$



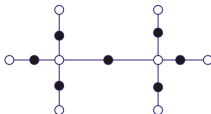
$\text{st}(T)^1$

¹J.J. Sylvester, Am. J. Math. 1 (1878) 64-104.

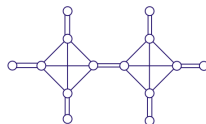
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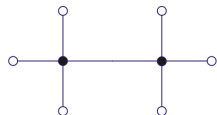


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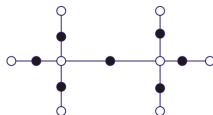
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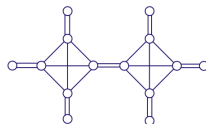
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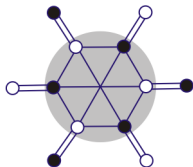
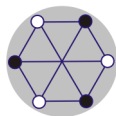


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- The median eigenvalues of a stellated tree satisfy $-1 \leq \lambda_L < 0 < \lambda_H \leq 1$.

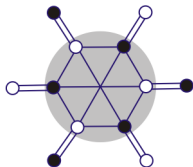
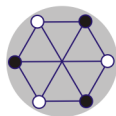
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Bounding Median Eigenvalues



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Bounding Median Eigenvalues

- (PISANSKI & FOWLER, 2010). Every tree with maximum degree at most 3 has median eigenvalues in $[-1, 1]$.

Bounding Median Eigenvalues

- (PISANSKI & FOWLER, 2010). Every tree with maximum degree at most 3 has median eigenvalues in $[-1, 1]$.
- (WU, YANG & Y., 2017+). Every bipartite graph with at most one perfect matching has median eigenvalues in $[-1, 1]$.

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- **PROBLEM:** Which graphs maximize HOMO-LUMO gap?
- **PROBLEM:** Which graphs have split spectrums?

THANK YOU!