Median Eigenvalues of Graphs

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(partly joint work with Behruz Tayfeh-Rezaie)

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Graph eigenvalues

G graph
vertex-set $V = V(G)$, edge-set $E = E(G)$, $n = |V|$

Adjacency matrix: $A = A(G) = (a_{uv})_{u,v \in V}$

where $a_{uv} = 1$ if $u \sim v$ and $a_{uv} = 0$ if $u \not\sim v$.

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Eigenvalue of G: eigenvalue of $A = A(G)$; $Ax = \lambda x$ $(x \neq \mathbf{0})$

All eigenvalues are real

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

and $\sum_{i=1}^{n} \lambda_i = 0$ (since $tr(A) = 0$).

Hückel theory

Hückel Theory: Eigenvalues of a molecular graph correspond to energy levels of electrons (two electrons per each energy level), and eigenvectors give descriptions of molecular orbitals.

Fowler & Pisanski (2010):

HL-index: $\boxed{R(G) = \max\{|\lambda_H|, |\lambda_L|\}}$

where $H = \lfloor \frac{n+1}{2} \rfloor$ and $L = \lceil \frac{n+1}{2} \rceil$.

Question: What is the largest value of $R(G)$ taken over all "chemically relevant graphs"?

Median eigenvalues of subcubic graphs

Subcubic graph: maximum degree ≤ 3

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Proof by combinatorial techniques and interlacing.

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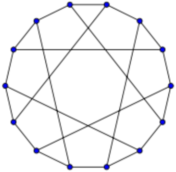
Heawood graph attains the maximum value, $R(H) = \sqrt{2}$.



Bipartite graphs

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$$\boxed{G \text{ has } \lceil cn \rceil \text{ median eigenvalues in } [-1, 1]}$$

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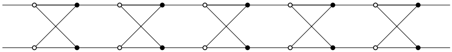
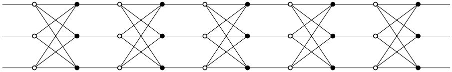
Theorem (Guo, M. 2013) $\exists$ infinitely many connected cubic bipartite graphs with $\boxed{R(G) = 1}$

Examples





$$\sigma(Z_k) = \{-1, 1\} \cup [k-1, k+1] \cup [-k-1, -k+1]$$

Two intervals, each with total spectral measure equal to $\frac{1}{2k}$

± 1, each have spectral measure equal to $\frac{1}{2} - \frac{1}{2k}$

Theorem (M., Tayfeh-Rezaie 2014+) G connected bipartite, max degree $\Delta \geq 3$. Then

$$\boxed{R(G) \leq \sqrt{\Delta - 2}}$$

except when G is the the incidence graph of a projective plane of order $\Delta - 1$, in which case $R(G) = \sqrt{\Delta - 1}$.

Proof - regular case

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- If $E = BB^T - kI$, then $\lambda_i(E) > -2 \quad \Rightarrow \quad E + 2I$ is PD
- Diagonal entries of $E + 2I$ are 2 $\quad \Rightarrow$
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- G connected $\quad \Rightarrow \quad H$ is connected
- Known fact: a connected regular graph with least eigenvalue > -2 is either K_n or C_n (with n odd). If $H = C_n$, then it is 2-regular and from $k^2 - k = 2$, we have $k = 2$, a contradiction. Hence, $H = K_n$

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- $H = K_n \quad \Rightarrow \quad G$ is the incidence graph of a projective plane of order $k-1$.

Construction by graph covers

- Construction of graphs with "almost" extreme median eigenvalues: For any integer k for which $k-1$ is a prime power, there exist infinitely many connected bipartite k-regular graphs G with $\sqrt{k-2}-1 < R(G) < \sqrt{k-1}-1$:

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- Recent breakthrough [A. Marcus, D.A. Spielman and N. Srivastava, Interlacing families I: Bipartite Ramanujan graphs of all degrees, arXiv:1304.4132]:
  and their proof of the Kadison-Singer Conjecture in Part II

  Control of λ_2 among new eigenvalues