Median Eigenvalues of Subcubic Graphs

Bojan Mohar

Simon Fraser University & IMFM

July 2013

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 $A = A(G)$; $Ax = \lambda x \quad (x \neq \mathbf{0})$

All eigenvalues are real

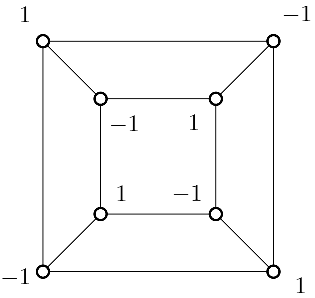
$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

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

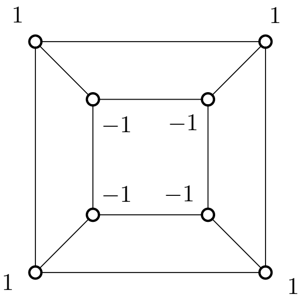
Examples

Characteristic equation: $Ax = \lambda x$

For each vertex v: $$\sum_{uv \in E} x_u = \lambda x_v$$



$\lambda = -3$



$\lambda = 1$

Overview of some applications

- Application 1: Google Page Rank
- Application 2: Expanders
- Application 3: Lovász ϑ-function
- Application 4: Hückel Theory
- Application 5: Wigner's Semi-Circle Law (random graphs)

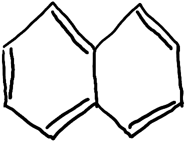
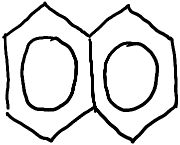
Summary

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq \lambda_{\lfloor n/2 \rfloor} \geq \cdots \geq \lambda_n$$

spectral gap
(expanders)

median eigenvalue
(HOMO-LUMO separation)

- chromatic number
- large independent sets
- ϑ-function

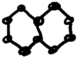
σ-bonds
σ-electrons
π-electrons

Hückel theory

(simplified Schrödinger equation for wave fn of π-electrons)

$\varepsilon_1, \varepsilon_2, \dots \varepsilon_n$ energy levels of π-electrons

$\varepsilon_i = a\lambda_i + b$

$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ eigenvalues of 

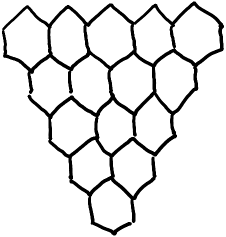
Eigenvectors correspond to molecular orbitals (MO).

HOMO - LUMO

Pauli principle: 2 π-electrons per energy level

$\lambda_{n/2}$ Highest Occupied MO (HOMO)

$\lambda_{n/2+1}$ Lowest Unoccupied MO (LUMO)

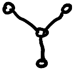


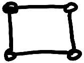
$n = 46$

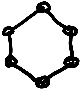
$\lambda_{23} = ?$

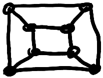
↑ median eigenvalue

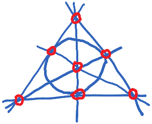
K_2  ± 1

$K_{1,3}$  $\pm\sqrt{2},\ 0^{(2)}$

C_4  $\pm 2,\ 0^{(2)}$

C_6  $\pm 2,\ \pm 1^{(2)}$

Q_3  $\pm 3,\ \pm 1^{(3)}$

H  Heawood graph

$\pm 3,\ \pm\sqrt{2}^{(6)}$

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

Theorem (M. 2012) G subcubic $\Rightarrow$ $\boxed{R(G) \leq \sqrt{2}}$

Proof by combinatorial techniques and interlacing.

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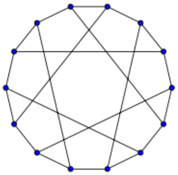
Heawood graph attains the maximum value, $R(H) = \sqrt{2}$.



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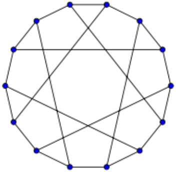


Question: Is Heawood graph chemically realizable as a pure carbon molecule (toroidal fullerene)?

Planar graphs

Theorem (M. 2012) G subcubic planar bipartite $\Rightarrow$ $\boxed{R(G) \le 1}$

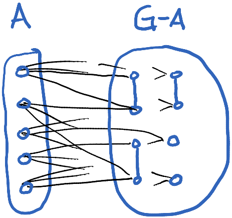
Conjecture. G subcubic planar $\Rightarrow$ $\boxed{R(G) \le 1}$

Many graphs attain this value (3-cube, C_6, K_2)

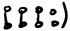
Eigenvalue Interlacing Theorem

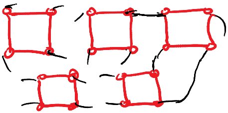
Theorem: $A \subseteq V(G)$, $|A| = k$, $1 \le i \le n-k$

$$\boxed{\lambda_{i+k}(G) \le \lambda_i(G-A) \le \lambda_i(G)}$$



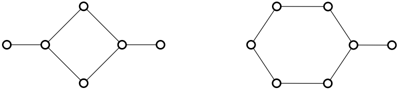
If $|A| < \frac{n}{2}$, then $\lambda_{n/2}(G) \le \lambda_1(G-A)$

$\lambda_1(G-A) = \lambda_1($  $) \le 1$

Bad news 

Proof by interlacing with additional tweak

Theorem (M. 2012) G subcubic planar bipartite $\Rightarrow$ $\boxed{R(G) \le 1}$



(a) (b)

(c) (d)

Why only planar graphs?

Why only planar graphs?

Theorem (M. 2013) G (connected) subcubic bipartite and not isomorphic to `Heawood` $\Rightarrow$ $\boxed{R(G) \leq 1}$

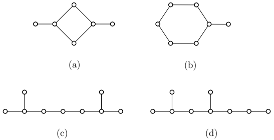
Theorem (M. 2013) $\exists c > 0$: $\forall G$ connected subcubic bipartite and not isomorphic to `Heawood` $\Rightarrow$

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

Main Lemma

G bipartite, (A, B) bipartition of $V(G)$

Increasing imbalance of (A, B): $C \subset A$ move to B, obtaining smaller set A' for which we can use $\lambda_{|A|}(G - A')$ in the interlacing theorem.



Theorem: $\forall G$ connected subcubic bipartite and not isomorphic to Heawood, then $\forall v \in V(G) \Rightarrow$
$B_{17}(v)$ contains a subset C that either increases imbalance of (A, B) or of (B, A)

Some open questions

- Is $R(d) = \sqrt{d}$ or $R(d) = \sqrt{d-1}$ or some value strictly between these.
- Is $R(d) = \widehat{R}(d)$ for every integer $d \geq 0$?
- If G is a subcubic graph of odd order, what is the maximum value of $|l_{H-1}|$ and $|\lambda_{H+1}|$? Examples of C_3 and C_5 show that $|\lambda_{H-1}|$ can be as large as 2 and λ_{H+1} can be as small as $-2\cos\frac{4\pi}{5} \approx -1.618$. However, there are only finitely many examples for which either $|\lambda_{H-1}| > \sqrt{2}$ or $|\lambda_{H+1}| > \sqrt{2}$.
- The proof of our theorem suggests that extremal graphs (e.g. those having maximum HL-index among d-regular graphs) must be close to be strongly regular. A similar property holds for graphs with maximum energy (Koolen-Moulton, Haemers). However, the graphs that are energy-extremal are not extremal for the HL-index. It remains an open problem to determine extremal examples for the HL-index.

Can we go any further?

Examples: Graph Fractals

Fractal-like constructions of cubic graphs give rise to examples with eigenvalues:

median eigenvalue 0 but no eigenvalues in the intervals $(0, \varphi - \varepsilon)$ or $(1 - \varphi + \varepsilon, 0)$ where $\varphi \approx 1.618$ is the golden ratio.