Spectral theory on combinatorial and quantum graphs

Topic 3: Operators on graphs and their spectra.

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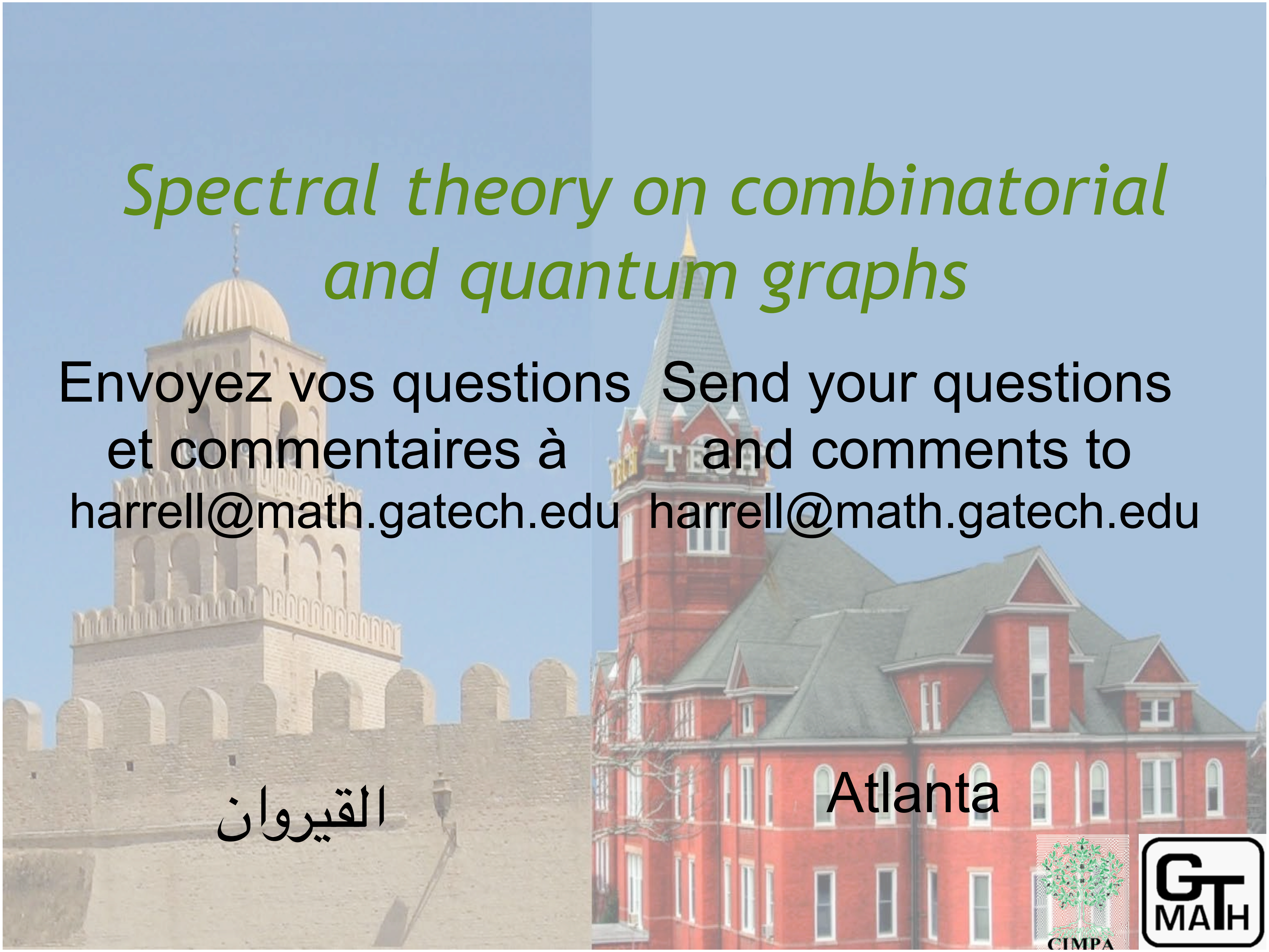
Spectral theory on combinatorial and quantum graphs
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The Laplacian on a graph

- The operator *d*d* is what we will define (up to a sign) as the *graph Laplacian*, $\mathcal{L}$ = - Δ = *d*d* = *Deg* - *A* . The quadratic form of $\mathcal{L}$ is:

$$\begin{aligned} \langle d^* df, f \rangle_{\mathcal{V}} &= \langle df, df \rangle_{\mathcal{E}} \\ &= \sum_{e \in \mathcal{E}} |f(t(e)) - f(s(e))|^2 \end{aligned}$$

Symmetric matrices that live on graphs

- The adjacency matrix A
- The graph Laplacian $\mathcal{L}$ = Deg – A = d*d
- The *renormalized graph Laplacian*

  $\mathrm{Deg}^{-1/2}\, \mathcal{L}\, \mathrm{Deg}^{-1/2}$ D = I - $\mathrm{Deg}^{-1/2}$ A $\mathrm{Deg}^{-1/2}$
- The *signless Laplacian*

  Q = Deg + A = BB*

Some matrices with additional structure

- A Schrödinger operator on a combinatorial graph can be defined as $\mathcal{L}$ + V, where V is a diagonal matrix on the vertex space, called the “potential energy.”
- Because the degree matrix is diagonal, it is often absorbed into V.
- Some physicists study these as discrete models of quantum systems.

Symmetric matrices that live on graphs

- These operators are trivially related for *regular* graphs, i.e., when every vertex has the same degree. However, when a graph is not regular, their relationship is more complex.

Some matrices with additional structure

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Some matrices with additional structure

- A *magnetic* Laplacian can be defined by including phase factors on the edges, such as in

  E(f) = $\sum_e |f(te) - e^{i\theta(e)} f(se)|^2$

  weights can also be included. Cf work by Sunada, Colin de Verdière - Torki, Lieb - Loss.

- Analogues of other differential operators, such as Dirac, cf. Golénia.

Can one "hear" the shape of a graph?

- Given the eigenvalues of one or other of these matrices, can you determine the structure of a graph? Of course we don't distinguish between graphs where we have just relabeled the vertices by a permutation.

Can one "hear" the shape of a graph?

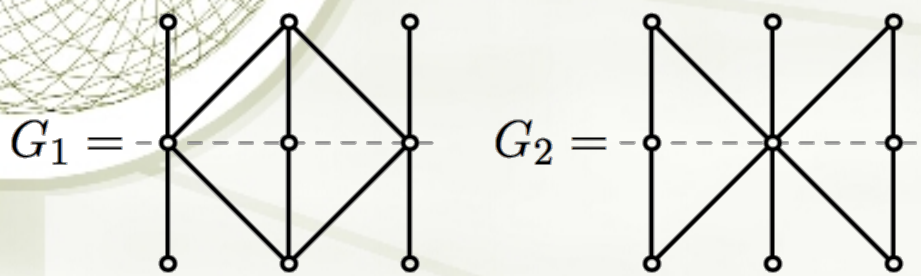
- There are only a finite number of possible n×n distinct adjacency matrices: ($2^{n(n-1)/2}/n!$ if you take permutations into account). Meanwhile, there is no obvious reason, or good theorem, restricting some eigenvalue, say the 2nd one, to a finite set you can define with a formula.
- So why not conjecture that the eigenvalues determine the graph?

Bad news - cospectral graphs

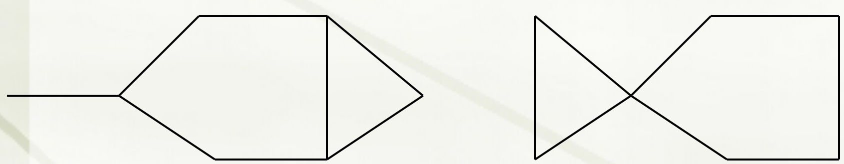
Definition. A *cospectral* (or isospectral) pair of graphs have precisely the same eigenvalues.

Cospectral graphs

Example of Steve Butler, Iowa State, for the “normalized Laplacian” and adjacency matrix.



Mouse and fish for the standard Laplacian.



There are various ways to describe a graph with a matrix, but in any version, the eigenvalues do not always determine the graph.

Cospectral graphs

- By the spectral diagonalization of matrices, a graph certainly *is* determined by the eigenvalues along with a basis of eigenvectors.
- Is there a good theorem about determining the graph from two spectra, as in Gel’fand-Levitan theory?

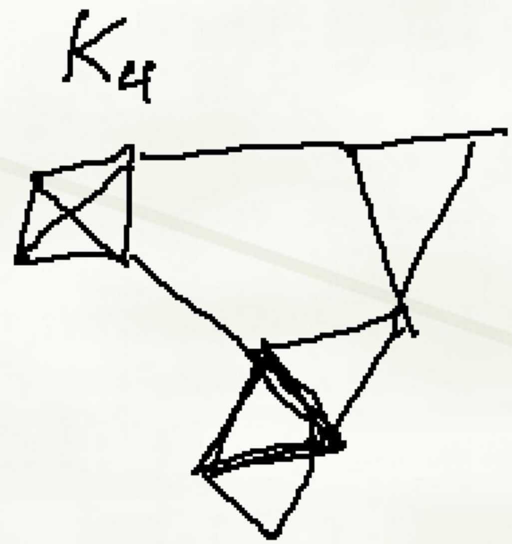
What would we like to "hear" about a graph?

- Basic features such as its size (numbers of vertices and edges, diameter) and topological properties like connectedness, cycles of various lengths, and measures such as the Zagreb index quantifying how closely connected vertices are.
- Clusters (= "communities"). How easily is a graph disconnected? If we set up a diffusive process, will it spend long times in some special subsets? Cf. the lectures by N. Anantharaman.

What would we like to "hear" about a graph?

- Colorings
- Numbers and locations of special subgraphs, such as "cliques" and spanning trees.
- For physical applications, counting functions and energies of eigenvalues.

- A “clique” is a complete graph, which is a subset of G.



What can one "hear" about a graph?

- Some elementary facts about eigenvalues of discrete graphs.
  - Let **1** be the vector of "all ones."

  We easily see that $\mathcal{L}$ **1** = **0**.
  - Is that the only eigenvector (up to multiples)?
  - Already from the weak form

$$E(f) = \sum_{e \in \mathcal{E}} |f(t(e)) - f(s(e))|^2$$

we can understand that the multiplicity of 0 is the number of connected components.

What can one "hear" about a graph? (we begin with the easy stuff)

- The number n of vertices is the same as the number of (not necessarily distinct) eigenvalues.
- The number m of edges is also easy to find by taking a trace or either $\mathcal{L}$ or A^2.

  Why?
- Think for a moment about A^k. What does the integer in the ij position tell us?
- The number of triangles is "audible."

Comments about traces…

- $tr(M) = \sum M_{vv}$

and also = sum of all eigenvalues.

Consider $M = A^2$. This matrix tells us how many "walks" of two steps there are from vertex u to v. If u=v, this is the same as the number of edges, i.e. the diagonals are the degrees d_v. But the sum of the degrees is 2 m (m=# edges), so we can "hear" the number of edges as ½ the sum of the squares of the eigenvalues of A.

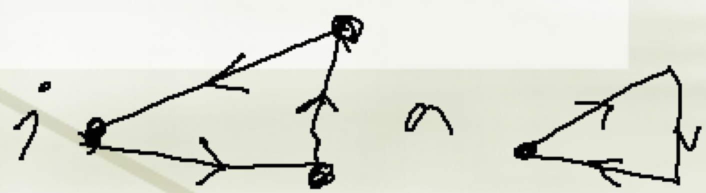
Comments about traces…

- Likewise, the diagonals of $\mathcal{L}$ are the degrees, so we also hear m via the formula

$$m = \tfrac{1}{2} \sum \lambda_i.$$

Comments about traces…

- Similarly, the diagonals of A^3 count the number of three-step walks from a vertex v to itself, which is twice the number of triangles touching v (clockwise and counterclockwise). When we take the trace, since each triangle touches three vertices, we overcount by a factor of 6:
- $T(G) = 6 \text{ tr } A^3$.



Comments about traces…

- Similar information can be obtained form the traces of powers of $\mathcal{L}$, but mixed with some other information, such as the Zagreb index:
- $\mathrm{tr}(\mathcal{L}^2) = \mathrm{tr}(\mathrm{Deg}^2 + A^2 - \sout{A\,\mathrm{Deg} - \mathrm{Deg}\,A})$

  $= \sum \lambda_i^2 + 2\,m.$

Comments about traces…

- Similar information can be obtained form the traces of powers of $\mathcal{L}$, but mixed with some other information, such as the Zagreb index:
- $tr(\mathcal{L}^3) = tr(Deg^3 - \sout{A\,Deg^2} - \sout{Deg^2 A} - \sout{Deg\,A\,Deg} + A^2\,Deg + A\,Deg\,A + Deg\,A^2 - A^3)$

  $= 4 \sum d_i^3 - 6\,T.$

Comments about traces…

- Is it easy to count other cycles? Unfortunately increasingly complex combinatorial questions arise in connecting the number of k-walks to the number of k-cycles, because a k-walk could contain some back-and-forth steps on edges, or, if k is not prime, multiple copies of cycles the lengths of which are divisors of k.

Hunting for eigenvalues

- If you can't find the eigenvalues of a self-adjoint operator exactly, you can search for them "variationally" in a number of ways, based on the spectral theorem:
  1. Approximate eigenvectors
  2. Min-max principles for individual eigenvalues
  3. Min-max principles for sums

Approximate eigenvectors

Suppose that $H = H^*$. Then $\lambda \in sp(H)$ iff there exists a sequence of "test functions" $\varphi_k \in \mathcal{D}(H)$, $\|\varphi\| = 1$, such that $\|(H - \lambda)\varphi_k\| \to 0$. The sequence $\{\varphi_k\}$ is referred to as an *approximate eigenvector*.

Approximate eigenvectors

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Suppose that λ is an isolated eigenvalue (possibly non-simple) of H and $\psi \in \mathcal{D}(H)$, $\|\psi\| = 1$, and let $\delta := \mathrm{dist}(\lambda, \mathrm{sp}(H) \setminus \lambda)$, and P be the spectral projector for λ. If $\|(H - \lambda)\psi\| \leq \delta' < \delta$, then

$$\|P\psi\|^2 \geq 1 - \left(\frac{\delta'}{\delta}\right)^2 .$$

$\lambda \in \sigma_p$ $\quad \varphi_n =$ e'vec. done.

otherwise suppose $(H-\lambda)\varphi_n \to 0$

$(H-\lambda)\varphi_n = \zeta_n \neq 0$

$$\frac{\|(H-\lambda)^{-1}\zeta_n\|}{\|\varphi_n\|} = \frac{1}{\text{sth} \to 0} \nearrow \infty$$

$\therefore (H-\lambda)^{-1}$ can not be bdd.

$\lambda \in \sigma(H)$ $\quad \chi_{(\lambda-\frac{1}{n},\lambda+\frac{1}{n})} \neq 0$

$\exists \varphi_n \in \operatorname{Ran} \chi_{(\lambda-\frac{1}{n},\lambda+\frac{1}{n})}$ $\|\varphi_n\| = 1$

$$\|(H-\lambda)\varphi_n\|^2 = \int_{\lambda-\frac{1}{n}}^{\lambda+\frac{1}{n}} (x-\lambda)^2 \, d\mu_{\varphi_n} < \frac{1}{n}$$

Min-max

Suppose that $H = H^* \geq CI$ for some $C > -\infty$ and that there are N eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ below the essential spectrum of H. For any $\mathfrak{M} \subset \mathfrak{H}$, define $\lambda(\mathfrak{M}) := sup \, \langle H\varphi, \varphi \rangle : \varphi \in \mathfrak{M}, \|\varphi\| = 1$. Set

$$\tilde{\lambda}_\ell := \inf\{\lambda(\mathfrak{M}) : \mathfrak{M} \subset \mathcal{D}(H), \dim(\mathfrak{M}) = \ell\}$$

for $\ell \leq N$. Then for all such ℓ, $\tilde{\lambda}_\ell = \lambda_\ell$.

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If H is a finite matrix related to some graph, one can apply min-max to –H, and get max-min characterizations of the eigenvalues counting from the top.

$$M_\ell = \text{span}\ \psi_1 \cdots \psi_\ell$$

$$P = \text{proj fn } M_{\ell-1}$$

In minmax $\dim M = \ell$ so $\exists\ f \in M \perp$

ran P = $Pf = 0$

$$\langle Hf, f\rangle = \sum_{k \geq \ell} \lambda_k |\langle f, \psi_k\rangle|^2 \geq \lambda_\ell \sum_{k \geq \ell} |\langle f, \psi_k\rangle|^2$$

$$\tilde{\lambda}_\ell \geq \lambda_\ell \quad \square$$

Courant

Courant-Weyl

$$\lambda_k^{\uparrow}(A) + \lambda_1^{\uparrow}(B) \leq \lambda_k^{\uparrow}(A+B) \leq \lambda_{k+1}^{\uparrow}(A) + \lambda_{n-1}^{\uparrow}(B)$$

(Another exercise from min-max)

Exercises.

1. Generalize the lemma showing that if the "residual" is small, the test function is nearly in the range of the spectral projector to the case where there is a narrow cluster of eigenvalues isolated from the rest of the spectrum by distance δ.

2. Show that it suffices in the min-max principle to have the test functions in the quadratic-form domain of H and to interpret $\langle H\varphi, \varphi\rangle$ as $E_H(\varphi)$.

3. Under the same circumstances as in the variational principle, suppose that $\{\phi_1, \dots, \phi_\ell, \ell \leq N$, is an orthonormal set of functions in the quadratic-form domain of H. Prove that

$$\sum_{j=1}^{\ell} \lambda_j \leq \sum_{j=1}^{\ell} E_H(\phi_\ell).$$

Playing around with the graph Laplacian

- Relationship with atomic edge Laplacians.
- Relationship with the complementary graph.
- Complete graphs and their eigenvectors.
- Some bounds on eigenvalues of graphs, revealing some of their properties.

Playing around with the graph Laplacian

- Relationship with atomic edge Laplacians. Note that

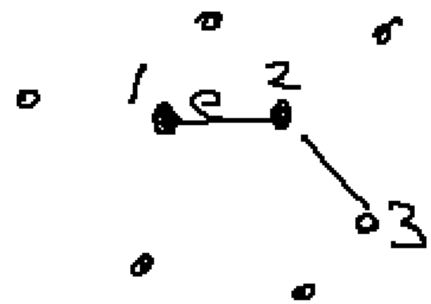
$$\mathcal{L}_G = \sum_{e \in \mathcal{E}(G)} \mathcal{L}_e$$

($\mathcal{L}_e$ is more properly $\mathcal{L}_e \oplus 0$.)

- This implies an interlacing theorem:

"Interlacing thm"

$$\mathcal{L} = \sum_{e \in E(G)} \mathcal{L}_e$$



$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \to sp(0, 2)$$

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \Big| \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Courant-Weyl

$$\begin{pmatrix} \begin{matrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{matrix} & 0 \\ 0 & 0 \end{pmatrix} \qquad \deg(0) = n-2$$

If add edge

min max $\quad \lambda_k(G+e) \geq \lambda_k(G)$

$\lambda_k(G+e) \leq \lambda_{k+1}(G)$

2nd largest e'val of

Playing around with the graph Laplacian

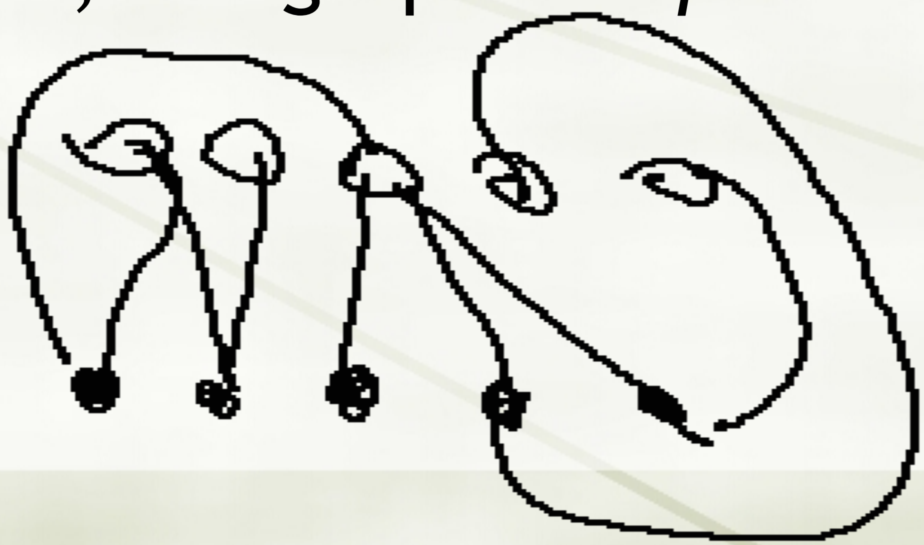
- Traces and degrees. The sum of the lowest k eigenvalues of $\mathcal{L}$ is bounded above by the sum of the lowest k d_v. Likewise, the sum of the highest k eigenvalues is bounded below by the sum of the highest k degrees.

Colorings?

- Is it possible that eigenvalues can be used to detect how many colors are needed so that each vertex can be labeled with a color, with no adjacent vertices of the same color?
- An efficient test for a 3-coloring is a major open problem, with implications for the study of algorithms.

Colorings?

- The minimal number of necessary colors is called the graph's *chromatic number*, $\chi(G)$.
- If $\chi(G)=2$, the graph is *bipartite*.



Spectral characterization of $\chi(G)=2$

- A graph is bipartite iff
  - 0 is an eigenvalue of the signless Laplacian Q
  - 2 is an eigenvalue of the renormalized Laplacian

1. These are equivalent:

If $C = I - Deg^{-1/2} A\, Deg^{-1/2}$ has eigenvalue 2,

then, multiplying by $Deg^{1/2}$,

$$A\, Deg^{-1/2}\, w + Deg^{1/2}\, w = 0.$$

With $u := Deg^{-1/2} w$, this reads $Q\, u = 0$.

Spectral characterization of $\chi(G)$=2

- A graph is bipartite iff
  - 0 is an eigenvalue of the signless Laplacian Q

2. Recalling that the weak form of the signless Laplacian is:

$$E_Q(f) = \sum_{e \in \mathcal{E}} |f(t(e)) + f(s(e))|^2$$

we see that if this is 0, then the eigenfunction f must have opposite values on every pair of u ~v. The sign of f_v gives a 2-coloring of G.

John Deven student at GT.

magnetic Laplacians

$$\sum_e \| f(s(e)) - e^{i\theta} f(t(e)) \|^2$$

$\Theta = \pi \Rightarrow Q = BB^*$

$\Theta = 0 \Rightarrow \mathcal{L}$

angle # Θ of pf.

conditions on which $\Theta \in$ sp

is equiv. to $\mathcal{L}$ (Lieb-Loss)

other properties of "Θ-laplacians"

Some references for discrete graphs and their spectra

- Y. Colin de Verdière, Spectres de graphes.
- D. Cvetković, P. Rowlinson, S. Simić, n Introduction to the Theory of Graph Spectra.
  - Warning! They number eigenvalues from greatest to least!
- T. Sunada, Discrete Geometric Analysis