Spectral theory on combinatorial and quantum graphs

Topic 3 (continued): Operators on graphs and their spectra.

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Where were we?

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:
- tr A^3= 6 T(G).

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:
- $\mathrm{tr}(\mathcal{L}^2) = \mathrm{tr}(\mathrm{Deg}^2 + A^2 -$ ~~A Deg – Deg A~~$)$

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

Some connections between spectra and the structure of a graph

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

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

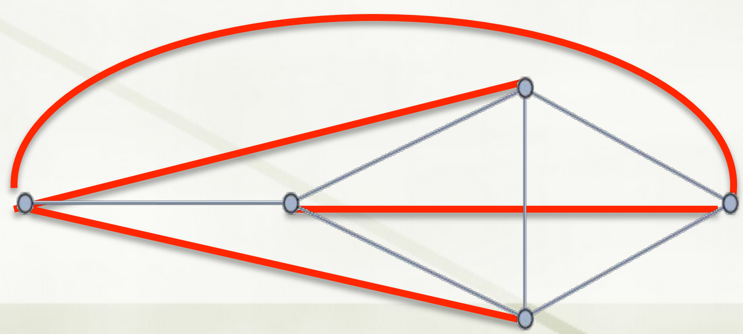
Playing around with the graph Laplacian

- 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

- If we add a graph and its complement, in the sense of including the edges of both, we get the complete graph K_n.

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$

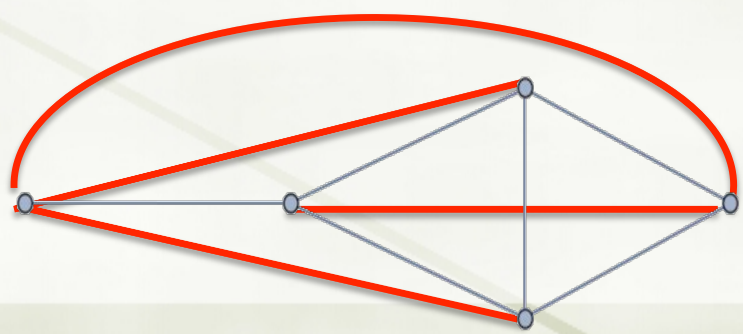


$$\begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Playing around with the graph Laplacian

- The complementary graph to G has edges connecting the pairs of vertices that are connected in G, and vice versa. The adjacency matrices differ off the diagonal by $0 \leftrightarrow 1$.

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$

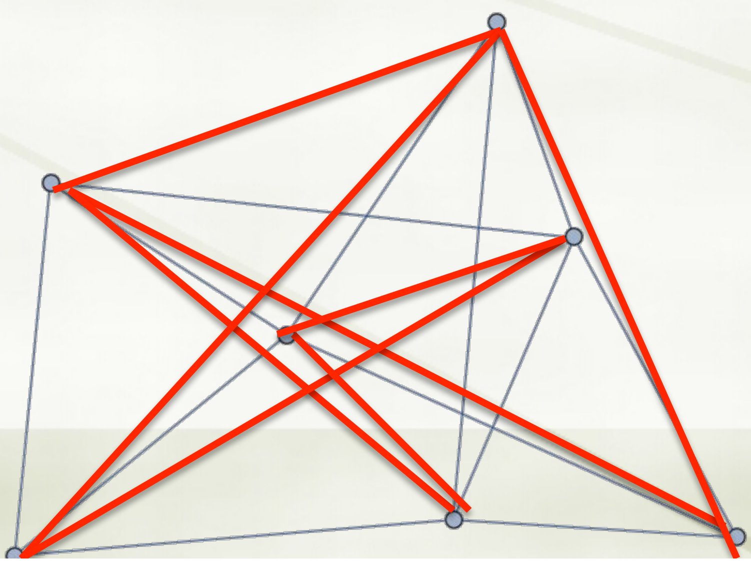


$$\begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Playing around with the graph Laplacian

- Another example

$$\begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 \end{pmatrix}$$



$$\begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Complete graph

What are the eigenvalues and eigenvectors? K_n is regular, so the eigenvectors will be the same for A, or Q.

$$\begin{pmatrix} 6 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 6 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 6 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 6 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 6 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & 6 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & 6 \end{pmatrix}$$

Playing around with the graph Laplacian

- The graph Laplacian of K_n is easy to analyze.

$$\begin{pmatrix} 6 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & 6 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 6 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 6 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 6 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & 6 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & 6 \end{pmatrix}$$

- It is of the form $n\,(I - P_1)$, where P_1 is the projector onto the vector **1**.

$$7 \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

$n(1 - \frac{P}{I})$ $\quad \vec{1} \to \vec{0}$

Suppose $f \perp \vec{1} \Rightarrow$ mean of f_u is 0

$\mathcal{L}$ considered as op on $\mathbb{C}^n - [\vec{1}]$

$\mathcal{L}_{K_n}$ $\quad nI$ on this set

$n-1$ times

$sp(\mathcal{L}_{K_n}) = \{0, n\}$

every vec $\perp \vec{1}$ is an e'vec.

Playing around with the graph Laplacian

- The graph Laplacian of the complete graph is easy to analyze.
- Every vector orthogonal to **1** is an eigenvector, with eigenvalue n.
- This is the maximal graph Laplacian: the spectrum of any graph Laplacian is in the interval [0,n].

Playing around with the graph Laplacian

- Thus the Laplacians of a graph and its complement are related by

$$\mathcal{L}_G + \mathcal{L}_{G^c} = n(I - P_{\mathbf{1}})$$

and if we work in the space of vectors $\perp \mathbf{1}$ we simply have

$$\mathcal{L}_{G^c} = nI - \mathcal{L}_G.$$

Playing around with the graph Laplacian

- It follows that *nonzero* eigenvalues of $\mathcal{L}_G$ and $\mathcal{L}_{G^c}$ are related by

$$\lambda \in sp(\mathcal{L}_G) \iff n - \lambda \in sp(\mathcal{L}_G^c)$$

and that they have the same eigenvectors!

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

Hunting for eigenvalues

- A good strategy is to use eigenvectors that relate to special graphs as test functions to study the graph at hand.
- An example of such a special graph is the complete graph.
- It has a cool "superbasis" of functions supported on individual edges.

The eigenvectors of the complete graph

The complete graph has a *tight frame* of nontrivial eigenfunctions consisting of functions equal to 1 on one vertex, -1 on a second, and 0 everywhere else. Let these functions be $h_{\mathbf{e}}$, where **e** is a directed edge (ordered vertex pair).

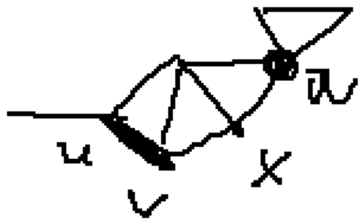
Variational bounds on graph spectra

Two facts are easily seen for vectors f of mean 0 (i.e. $\perp \mathbf{1}$) :

1. $$\langle \mathcal{L} h_{\overrightarrow{uv}}, h_{\overrightarrow{uv}} \rangle = d_u + d_v + 2a_{uv}$$

2. $$\sum_{\mathbf{e} \in \overrightarrow{\mathcal{E}}} |\langle h_{\mathbf{e}}, f \rangle|^2 = 2(n-1)\|f\|^2$$

$$h_{\vec{uv}} = \begin{cases} 1 & \text{on } u \\ -1 & \text{on } v \\ 0 & \text{otherwise} \end{cases} \qquad h_{\vec{uv}}(w)$$



$$\mathcal{L} h_{\vec{uv}} = 0 \quad w \nsim e$$

$$\mathcal{L} h_{\vec{uv}}(x) = +1 \qquad \mathcal{L} h_{\vec{uv}}(u) = d_u + 1$$

Gen pattern is

$$\delta_u(w) = \begin{cases} 0 & \text{if } w \neq u \\ 1 & \text{if } w = u \end{cases}$$

$$\mathcal{L} h_{uv}(w) = d_u \delta_u - d_v \delta_v + \vec{A}_{\cdot v} - \vec{A}_{\cdot u}$$

Var calcs $\langle h_{uv}, \mathcal{L} h_{uv} \rangle$

$$f \perp \vec{1} \Rightarrow \qquad \langle h_{\overrightarrow{uv}}, f h_w \rangle \text{ simple}$$

$$\sum |\langle h_{\overrightarrow{uv}}, f h_{uv} \rangle|^2 = C \|f\|^2$$

"tight frame"

$C = 2(n-1)$

Variational bounds on graph spectra

The “averaged variational principle” for sums of eigenvalues eliminates the need for orthogonalization.

The averaged variational principle

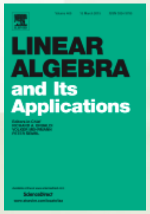
$$\frac{1}{k}\sum_{j=0}^{k-1}\mu_j \leq \frac{1}{|\mathfrak{M}_0|}\int_{\mathfrak{M}_0} \frac{Q_M(f_\zeta, f_\zeta)}{\|f_\zeta\|^2}\,d\sigma$$

where

$$\int_{\mathfrak{M}} \frac{|\langle \phi, f_\zeta\rangle|^2}{\|f_\zeta\|^2}\,d\sigma = A\|\phi\|^2$$

for a fixed constant $A > 0$, *and* $\mathfrak{M}_0 \subset \mathfrak{M}$ *such that* $|\mathfrak{M}_0| \geq kA.$

Harrell-Stubbe LAA, 2014

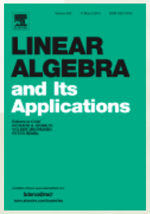


The averaged variational principle

$$\frac{1}{k}\sum_{j=0}^{k-1}\mu_j \leq \frac{1}{|\mathfrak{M}_0|}\int_{\mathfrak{M}_0} \frac{Q_M(f_\zeta, f_\zeta)}{\|f_\zeta\|^2}\, d\sigma$$

Averages within averages!

Harrell-Stubbe LAA, 2014



Variational bounds on graph spectra

From the averaged variational principle,

$$\sum_{j \le L} \lambda_j \le \frac{1}{2n} \min_{\text{choices of nL pairs}} \sum_{uv} (d_u + d_v + 2a_{uv})$$

Variants

For the normalized graph Laplacian,

$$\sum_{j=1}^{k-1} \mathfrak{c}_j \leq \frac{1}{4m} \sum_{\mathfrak{M}_0} (d_u + d_v + 2a_{uv}),$$

Variants

Corollary 9 *Let G be a finite connected graph on n vertices. Then for $1 \leq k < n-1$, the eigenvalues $\alpha_0 \geq \alpha_1 \geq \cdots \geq \alpha_{n-1}$ of the adjacency matrix A_G satisfy the elementary inequalities*

$$\sum_{j=0}^{n-k-1} \alpha_j \geq \min\left(k, \left\lfloor \frac{2m}{n} \right\rfloor\right),$$
$$\sum_{j=n-k}^{n-1} \alpha_j \leq -\min\left(k, \left\lfloor \frac{2m}{n} \right\rfloor\right). \qquad (3.25)$$

Now let $\{\alpha_{\ell_j}\}$, $\ell = 0, \ldots, n-1$ denote the eigenvalues α_j reordered by magnitude, so that $|\alpha_{\ell_0}| \leq |\alpha_{\ell_1}| \leq \ldots$. Then for any set $\mathfrak{M}_0$ of nk ordered pairs of vertices,

$$\sum_{j=0}^{k-1} \alpha_{\ell_j}^2 \leq \frac{1}{2n} \sum_{(u,v)\in\mathfrak{M}_0} (d_u + d_v - 2(A^2)_{uv}). \qquad (3.26)$$

Challenges for the future

- Spectral conditions to determine a graph uniquely (up to permutations). Are there two independent spectra that accomplish this?
- How many different graph spectra are there, and what “universal” constraints characterize the possible spectra?
- Where do the eigenfunctions concentrate? Are there explicit bounds that reflect this?

Spectral theory on combinatorial and quantum graphs

Topic 4 Introduction to quantum graphs.

CIMPA

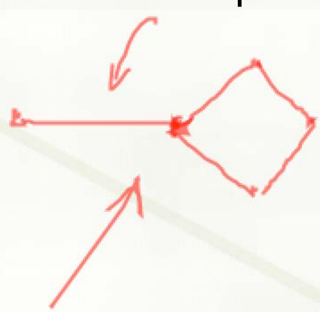
GT MATH

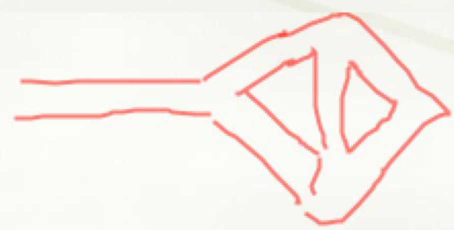
What is a quantum graph?

- We now allow the edges to be intervals, on which something interesting happens. (I.e., a differential equation!)

Microelec circuit

Schr. eq





How do we connect at verts?

What is a quantum graph?

- We now allow the edges to be intervals, on which something interesting happens. (I.e., a differential equation!)
- There are many choices, but I will only discuss Schrödinger equations:

$$-\psi'' + V(x)\,\psi = \lambda\,\psi$$

What is a quantum graph?

- Edge lengths can vary, and can be infinite. (For technical reasons we assume that every edge has length $\geq \delta$ for some fixed $\delta > 0$. The important new feature is that the edges are connected at vertices. What conditions do we impose there?

Cont at v.

- Again, there are many choices, but we mostly choose "Kirchhoff" or "Neumann" conditions,

$$\sum_{e \sim v} f_e'(v^+) = 0$$

What is a quantum graph?

- The Sobolev space $H^1(G)$ for a quantum graph is defined by completing the continuous, compactly supported functions in the Sobolev norm obtained from an orthogonal sum of Hilbert spaces of the form

$$\bigoplus_{e\in\mathcal{E}} H^1(e, ds)$$

where ds is the arclength on the edge.

What is a quantum graph?

- The functions in $H^1(G)$ are continuous at the vertices (i.e., up to equivalence classes).
- The weak form of the quantum graph is

$$f \in H^1(G) \to \sum_{e \in \mathcal{E}} \int_e (|f'(x_e)|^2 + V(x)|f(x_e)|^2) dx_e.$$

- To avoid some technical issues, we'll assume that V(x) ≥ C > - ∞ and continuous.

What is a quantum graph?

- If f is C^2 on each edge, and we integrate this by parts, we get

$$\sum_{e \in \mathcal{E}} \int_e (-f''(x_e) + V(x_e)f(x_e))\overline{f(x_e)}dx_e.$$

provided that the Kirchhoff conditions apply. (Otherwise there are boundary terms.) We write this as <Hf , f> .

Illustrative examples

1. An interval, V = 0.
   - But let's pretend that there is a vertex in the middle!

eig eq?

$-\psi'' = \lambda\psi$ $\lambda = k^2$

$\cos\left(\ell(1+x)\frac{\pi}{2}\right)$ $\left(\frac{\pi}{2}\right)^2\ell^2 = \lambda$

$k = \frac{\pi\ell}{2}$

$-1 \le x \le 1$

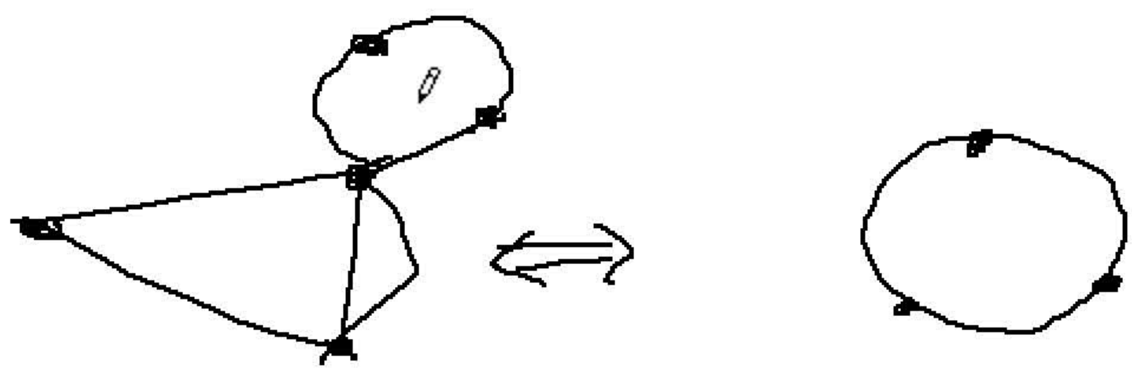
K ends?

± 1 K $\Leftrightarrow$ $f'(\pm 1) = 0$ Neuman BC.

$$f'(0^+) - f'(0^-) = 0 \Longleftrightarrow f' \text{ cont at } 0$$

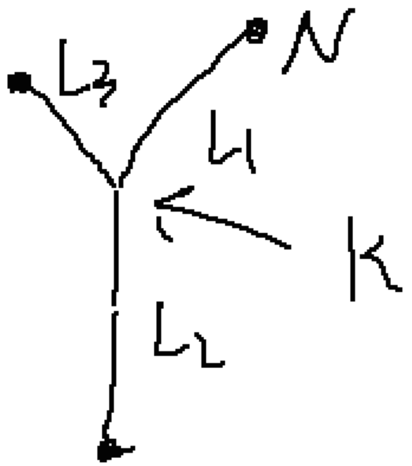
effectively a d_2 vertex

does nothing!



Illustrative examples

2. The regular Y-graph, V = 0.



$\frac{\psi'}{\psi}$ satifies k (on $\psi = 0$)

$$\sum_{e \sim v} \frac{\psi_e'(v)}{\psi_e} = 0$$

efns on e's are $\cos(k(L_\ell - x_\ell))$

$$k \Rightarrow \sum_\ell k \tan(k L_\ell) = 0$$

This is a trans eq

$$\boxed{\sum_\ell \tan(k L_\ell) = 0}$$

k_j solve this eq.

(∞ # frem $\to \infty$)

What happens when you…

- Add or increase an edge? (Say, when V=0)?
- Identify two vertices? √
- Impose a Dirichlet condition on a vertex?

Interlacing thms

$$\sum_e \int_e |f'|^2 + V|f|^2 \quad + \text{ cont.}$$

Change graph in various ways

$$\lambda_k \le \tilde{\lambda}_k \le \lambda_{k+1}$$

Identify them.

$\lambda_k \uparrow$? $\lambda_k \downarrow$?

λ_k min max

$$= \inf_{\substack{\text{subst } M \\ \dim k}} \sup \langle f, Hf \rangle \qquad \underset{\text{satisfy conds}}{\|f\| = 1}$$