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...

\[ \text{tr}(M) = \sum M_{vv} \]

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 \( 2m \) (\( m=\# \text{ edges} \)), so we can “hear” the number of edges as \( \frac{1}{2} \) the sum of the squares of the eigenvalues of \( A \).
Likewise, the diagonals of $\mathcal{L}$ are the degrees, so we also hear $m$ via the formula

$$m = \frac{1}{2} \sum \lambda_i.$$
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:

$$\text{tr } A^3 = 6 \ T(G).$$
Similar information can be obtained from the traces of powers of \( \mathcal{L} \), but mixed with some other information, such as the Zagreb index:

\[
\text{tr}(\mathcal{L}^2) = \text{tr}(\text{Deg}^2 + A^2 - A \text{Deg} - \text{Deg} A) = \sum d_i^2 + 2 m.
\]
Some connections between spectra and the structure of a graph

- Similar information can be obtained from the traces of powers of $\mathcal{L}$, but mixed with some other information, such as the Zagreb index:

\[
\text{tr}(\mathcal{L}^3) = \text{tr}(\text{Deg}^3 - A \cdot \text{Deg}^2 - \text{Deg}^2 \cdot A - \text{Deg} \cdot A \cdot \text{Deg} + A^2 \cdot \text{Deg} + A \cdot \text{Deg} \cdot A + \text{Deg} \cdot A^2 - A^3)
= 4 \sum d_i^3 - 6 T.
\]
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 $K_n$. 

\[
\begin{pmatrix}
0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 1 \\
0 & 0 & 1 & 0 & 1 \\
0 & 1 & 1 & 1 & 0
\end{pmatrix}
\quad
\begin{pmatrix}
0 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0
\end{pmatrix}
\]
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
Playing around with the graph Laplacian

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

\[
\begin{pmatrix}
6 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & 6 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & 6 & -1 & -1 & -1 & -1 \\
-1 & -1 & -1 & 6 & -1 & -1 & -1 \\
-1 & -1 & -1 & -1 & 6 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & 6 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & 6
\end{pmatrix}
\]
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.

$$
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix} = 
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}
$$
\[ \frac{n(1-P_i)}{I} \rightarrow 0 \]

Suppose \( I \rightarrow \infty \) the mean of \( f_n \) is 0

Let consider \( \omega \) on \( C^n \setminus \{i\} \)

Let \( n \) be this set \( \mathbb{N} \cap n \) on this set \( \sum_{n=1}^{\infty} \frac{1}{n^2} \)

Every vector \( I \) is an eigenvector.
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

$$\mathcal{L}_G + \mathcal{L}_{G^c} = n(I - P_1)$$

and if we work in the space of vectors 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

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

and that they have the same eigenvectors!
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
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 $h_e$, 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. \( \langle f \rangle = 0 \)):

1. \[ \langle \mathcal{L} h_{u \rightarrow v}, h_{u \rightarrow v} \rangle = d_u + d_v + 2a_{uv} \]

2. \[ \sum_{e \in \bar{E}} | \langle h_e, f \rangle |^2 = 2(n - 1) \| f \|^2 \]
\[ h_{uv} = \begin{cases} 1 & u = v \\ -1 & \text{otherwise} \\ 0 & \end{cases} \]

\[ \sum_{uv} h_{uv} = 0 \quad \forall x \in X \]

\[ \sum_{uv} h_{uv}(x) = +1 \quad \exists h_{uv}(x) = d_u + v \]

Gen pattern is

\[ S_u(w) = \begin{cases} 0 & \text{if } w \neq u \\ 1 & \text{if } w = u \end{cases} \]

\[ \sum_{uv} h_{uv}(w) = d_u S_u - d_v S_v + \overrightarrow{A_{uv}} - \overrightarrow{A_{vu}} \]

Var calc: \[ \langle h_{uv}, x h_{uv} \rangle \]
\[ f^T I = \langle h_{\mu\nu}, R h_{\mu\nu} \rangle \text{ simple} \]

\[ \sum K(h_{\mu\nu}, f h_{\mu\nu})^2 = C \|f\|^2 \]

"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

\[ \frac{1}{k} \sum_{j=0}^{k-1} \mu_j \leq \frac{1}{|M_0|} \int_{M_0} \frac{Q_M(f_{\zeta}, f_{\zeta})}{\|f_{\zeta}\|^2} \, d\sigma \]

where

\[ \int_{M_0} \frac{|\langle \phi, f_{\zeta} \rangle|^2}{\|f_{\zeta}\|^2} \, d\sigma = A\|\phi\|^2 \]

for a fixed constant \( A > 0 \), and \( M_0 \subset M \) such that \( |M_0| \geq kA \).
The averaged variational principle

\[
\frac{1}{k} \sum_{j=0}^{k-1} \mu_j \leq \frac{1}{|M_0|} \int_{M_0} \frac{Q_M(f_\xi, f_\xi)}{\|f_\xi\|^2} \, d\sigma
\]

Averages within averages!

Harrell-Stubbe LAA, 2014
Variational bounds on graph spectra

From the averaged variational principle,

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

For the normalized graph Laplacian,

\[
\sum_{j=1}^{k-1} c_j \leq \frac{1}{4m} \sum_{m_0} (d_u + d_v + 2a_{uv}),
\]
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

\[
\sum_{j=0}^{n-k-1} \alpha_j \geq \min \left( k, \left\lfloor \frac{2m}{n} \right\rfloor \right),
\]

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

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

\[
\sum_{j=0}^{k-1} \alpha_{\ell_j}^2 \leq \frac{1}{2n} \sum_{(u,v) \in \mathcal{M}_0} (d_u + d_v - 2(A^2)_{uv}).
\] (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.
What is a quantum graph?

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

How do we connect at verts?

Schr. eq

Microelec circuit
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?

- 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

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

- To avoid some technical issues, we’ll assume that $V(x) \geq C > -\infty$ and continuous.
What is a quantum graph?

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

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

provided that the Kirchhoff conditions apply. (Otherwise there are boundary terms.) We write this as $<Hf, f>$. 
1. An interval, $V = 0$.
   - But let’s pretend that there is a vertex in the middle!

\[
\psi'(r) = \chi \psi \\
\cos(\lambda (1 + \frac{1}{2} + \frac{\pi}{2})) \\
\lambda = k^2 \\
\frac{\hbar^2 k}{\mu} = \lambda \\
k = \frac{\pi k}{2}
\]
\[-1 \leq x \leq 1\]

K \text{conds?}

\[ f'(x) \neq 0 \text{ Neumann BC.} \]

\[ f'(0^+) - f'(0^-) = 0 \iff f' \text{ cont at } 0 \]

effectively a \( d_2 \) vertex

does nothing!

\[ \text{diag} \leftrightarrow \text{circle} \]
Illustrative examples

2. The regular Y-graph, $V = 0$. 
$$\psi' = \text{Satisfy } k \quad (a \psi = 0)$$

$$\sum_{\text{spec}} \frac{\psi'_r u^4}{\psi_x} = 0$$

Efran on $c$'s on $\cos \left( k \left( L_e - x \right) \right)$

$$k \Rightarrow \sum k \tan \left( k L_e \right) = 0$$

This is a trans eq.

$k_j$ solve this eq.

$$\sum \tan \left( k L_e \right) = 0$$

(00 ≠ from ̂∞).

$k_j$ solve this eq. (ab ≠ from ̂∞).
What happens when you...

- Add or increase an edge? (Say, when \( V=0 \))?
- Identify two vertices? √
- Impose a Dirichlet condition on a vertex?
Interlacing thus
\[ \sum_{\mathbf{x}} \left| \mathbf{H}^2 \mathbf{x} + \mathbf{V} \mathbf{f} \right|^2 \] 
and
\[ \text{cont.} \]

Change graph in various ways

\( \lambda_k \leq \lambda_{k+1} \) ?

Identify them.

\( \lambda_k \leq \lambda \) ?

\( \lambda_k \leq \min \text{ max} \)

\( = \inf \sup \langle \mathbf{f}, \mathbf{H} \mathbf{f} \rangle \)

Satisfies cond 3