SPECTRAL THEORY ON COMBINATORIAL AND QUANTUM GRAPHS

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Abstract. These lecture notes were developed for a minicourse at the CIMPA School in Kairouan, Tunisia, in November, 2016. Videos and pdfs of the lectures are available at
http://www.mathphysics.com/harrell/pub/Kairouan/.

Spectral theory on graphs is an active and well-developed subject, and these few lectures can be but an invitation to the student, who can learn much more by reading some of the monographs in the references. Here I have tried to hit a few highlights of the theory of both discrete and quantum (metric) graphs, and to draw attention to some research topics that may be in reach at this time. Inevitably the selection reflects the author's personal taste and is idiosyncratic.

1. The Ubiquitous Laplacian.

Our first topic is the Laplace operator, which makes an appearance in physical models from vibration theory to quantum mechanics, and in mathematical fields from probability to analytic function theory. It is virtually everywhere, a ubiquitous part of our mathematical understanding of the world. But why? What makes it ubiquitous?

Most familiarly, if we have a real second-order elliptic partial differential equation, and it is invariant under translations and unitary transformations of the space, its leading-order part must be a constant multiple of the Laplacian. To see this, recall that the leading-order part of such a PDE can always be written as

$$\sum_{i,j} \frac{\partial}{\partial_i} A_{ij}(x) \frac{\partial}{\partial_i} u,$$

where the matrix-valued function A can be assumed symmetric, because $\frac{\partial^2 u}{\partial_i \partial_j} = \frac{\partial^2 u}{\partial_j \partial_i}$. Now, translation-invariance implies that A is independent of x, and the symmetry of A allows it to be diagonalized by a certain choice of coordinate axes. Since interchanging any pair of coordinates is a unitary

symmetry of the Euclidean space, the diagonal version of A must have the same value at every entry of the principal diagonal. Hence A is a constant multiple of the identity, which means that the leading-order part of the PDE is the Laplacian, up to this multiple.

What happens when we lose these symmetries, when we consider operations on a surface, or on a manifold? The essence of a manifold is that it looks locally like Euclidean space. In fact, if you single out a given point, you can find coordinates, called *Fermi coordinates*, in which the metric tensor at that spot becomes the identity, just as for Euclidean space. Of course, it does this only momentarily. Think, for example of the sphere, with spherical coordinates θ, ϕ, for which

$$\begin{aligned} x &= rsin\theta \cos\phi \\ y &= rsin\theta \sin\phi \\ x &= r\cos\theta. \end{aligned}$$

As we know, fixing $r = 1$, the arc length and Laplacian look like:

$$ds^2 = d\theta^2 + \sin^2\theta d\phi^2$$

$$\Delta = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\phi^2},$$

but on the equator, where $\sin\theta = 1$ and its derivative is zero, we obtain the familiar Laplacian as the unweighted sum of the second derivatives with respect to an orthogonal coordinate system.

One could approach the Laplace-Beltrami operator by using Fermi coordinates at some special point, at which the Laplacian is proclaimed to have the Euclidean form, and then calculating the complications that arrive as soon as one moves avay from the special point. Instead of following this circuitous route, however, let us begin with the *weak form* of the Laplace operator, which is the quadratic form on a domain or manifold Ω defined by

$$(f,g) \to \int \nabla f \cdot \overline{\nabla g}\, dVol = \int f(-\Delta)\overline{g}\, dVol + \text{possible boundary contribs.}$$

Ordinarily, if there is a boundary, the preference is to make the boundary contributions vanish by imposing appropriate boundary conditions, when defining the Laplacian as a proper self-adjoint operator, but here we shall be more concerned with the quadratic form than the operator. (For the precise definition of self-adjoint differential operators, and in particular how to pass from the weak form to the operator via the Friedrichs extension, see the lectures by Najar or monographs such as [1, 40, 41, 44].)

As a further simplification, observe that by the *polarization identity* it suffices to consider the quadratic form with the simplification that $f = g$, that is,

$$f \to E(f) := \int |\nabla f|^2 \, dVol. \tag{1}$$

Verification Exercise. Show the validity of the polarization identity,

$$\int \nabla f \cdot \overline{\nabla g} = \frac{1}{4}\Big(E(f+g) - E(f-g) + iE(f+ig) - iE(f-ig) \Big).$$

Again, among all quadratic expressions in the first derivatives of f, the integrand in (1) is singled out, up to a constant multiple, as the unique choice with the simplest form. The infamously complicated form of the Laplace-Beltrami operator in terms of a metric tensor,

$$\Delta_{LB} f := \sum_{ij} \frac{1}{\sqrt{g}} \partial_i g^{ij} \sqrt{g} \partial_i f, \tag{2}$$

where $g := \det(g_{ij})$, is simply what you obtain if you introduce local coordinates and integrate (1) by parts, noting that the metric makes an appearance in the expression for the volume element:

$$\int |\nabla f|^2 \, dVol = \int \overline{f}(-\Delta_{LB} f) \, d\mathrm{Vol} + \text{possible boundary contribs.} \tag{3}$$

Verification Exercise. Verify (2), (1).

You are, however, advised to avoid (2) at all costs if you can accomplish your goal with (1)!

Summarizing our first point of view:

• **The Laplacian is the most symmetric differential operator of second order.**

Another point of view on the Laplacian is probabilistic. Here we could begin by thinking about the normalized Gaussian probability distribution:

$$P(x, y, t) := \frac{1}{(\pi 4t)^{\frac{d}{2}}} \exp(-|x-y|^2/4t). \tag{4}$$

(The coefficients of 4 multiplying the time t are unnecessary but give rise to some convenient normalizations.)

By convolution, the functions P define a one-parameter semigroup, i.e., for any bounded, continuous function f, $[\mathbb{P}_t f](x) := \int P(x, y, t) f(y) dy$ has the following properties:

(1) $lim_{t\to 0}\mathbb{P}_t = \mathbb{I}$
(2) $\mathbb{P}_t\mathbb{P}_s = \mathbb{P}_s\mathbb{P}_t = \mathbb{P}_{t+s}$.

The procedure of convolution with a Gaussian distribution is familiar in many contexts, from information theory, where it represents loss of information due to random events, to diffusion, to image analysis, where it is used to smooth and blur an image.

In semigroup theory, the *infinitesimal generator* refers to the derivative of the semigroup at $t = 0$, which turns out to be ..... the Laplacian. For all $t > 0$, P satisfies the heat equation, $\frac{\partial P(x,y,t)}{\partial t} = \Delta_x P(x, y, t) = \Delta_y P(x, y, t)$.

Verification Exercise. Verify all of the claims made about $\mathbb{P}_t$.

Summarizing the probabilistic origins of the Laplacian:
• **The Laplacian is the generator of the most natural diffusion process.**

With this in mind, if we are not studying a Euclidean space but a manifold, a graph, or some other structure, and we set up a diffusion process that is as symmetric and simple as possible, then we could use the generator of the associated semigroup to define a Laplacian.

Let us next consider a basic question of analysis: How does a quantity compare with its average value?

Suppose that a sufficiently smooth function f is defined on some Euclidean set. Let us define its average over nearby spheres of radius r as

$$F(x, r) := \langle f\rangle_{\mathbb{S}_r(x)} = \frac{1}{d\ \omega_d\, r^{d-1}} \int_{|y-x|=r} f(y) d^{d-1}y, \tag{5}$$

where the volume of the $d-1$-dimensional sphere of radius r has been expressed in terms of the volume of the unit ball in d dimensions,

$$\omega_d := \frac{\pi^{\frac{d}{2}}}{\Gamma\left(1+\frac{d}{2}\right)}.$$

For now x is simply fixed. If f is continuous at x, then clearly $\lim_{r\downarrow 0} F(x, r) = f(x)$. But how do the two quantities deviate from each other when $r > 0$? We can differentiate with respect to r as follows. First rewrite $F(x, r)$ as an integral over the unit sphere, as

$$F(x, r) = \frac{1}{d\ \omega_d} \int_{\mathbb{S}^{d-1}} f(x + r\alpha) d^{d-1}\alpha, \tag{6}$$

because of which

$$\begin{aligned}\frac{\partial F(x,r)}{\partial r} &= \frac{1}{d\ \omega_d}\int_{\mathbb{S}^{d-1}} \alpha\cdot\nabla f(x+r\alpha)d^{d-1}\alpha \\ &= \frac{1}{d\ \omega_d\, r^{d-1}}\int_{|y-x|=r} n\cdot\nabla f(y)d^{d-1}y \\ &= \left(\frac{r}{d}\right)\frac{1}{\omega_d\, r^d}\int_{|y-x|\le r}\nabla\cdot\nabla f(y)d^d y,\end{aligned}$$

according to the divergence theorem. We thus have the exact formula

$$\frac{\partial \langle f\rangle_{\mathbb{S}_r(x)}}{\partial r} = \left(\frac{r}{d}\right)\langle \Delta f\rangle_{\mathbb{B}_r(x)}\,, \tag{7}$$

and if we check the derivation for the degree of regularity needed, we see that this formula is valid for any function with absolutely continuous gradient. In summary, the remarkable formula (7) tells us that:

• **The Laplacian measures how a function differs from its nearby averages.**

Formula (7) further implies some familiar facts related to the Laplacian, especially the mean-value property.

By one definition, a *subharmonic* function is one whose value at x is always less than or equal to its nearby averages over balls of radius r centered at x, while a *superharmonic* function is the negative of a subharmonic function. (A harmonic function is both subharmonic and superharmonic.) If $\Delta f \ge 0$, Eq. (7) leads easily to a proof that f is subharmonic. From the subharmonic property, the maximum principle is a further consequence: On any connected open set, if a subharmonic function has an interior maximum, then it is constant.

Exercise. Formally prove the maximum principle for harmonic functions. (Eq. (7) and its applications for PDE are further discussed in the textbook [25].)

The alert student will have appreciated that the probabilistic and averaging characterizations of the Laplacian make no mention of the differentiability of a function with respect to x. For this reason, they can be used to define Laplacians in measure-theoretic settings on sets lacking sufficient smoothness to differentiate, for example fractals, and in that sense are more satisfying and broadly applicable than the definitions requiring classical differentiation. They also point the way to the notion of a Laplacian on a graph.

2. Graphs and the operators living on them

In this section I briefly provide a framework for understanding the analogues of concepts of analysis and geometry in the setting of networks, which are usually called *graphs* in the mathematical literature. We consider first the case of discrete, or combinatorial, graphs and later quantum graphs. For a good textbook on the theory of graphs, see [10] or [23]. Here I shall comment on how to adapt the concepts of analysis and geometry to graphs. The reader who wishes to go more deeply into the subject of analysis on graphs is advised to look into the work of Sunada [43].

A graph consists of a vertex set $\mathcal{V}$, thought of as points, and an edge set $\mathcal{E}$, which can be identified with a subset of pairs of vertices, considered as *connected*. When u is connected to v we write $u \sim v$, and likewise when an edge e is connected to a vertex v we write $v \sim e$ or equivalently $e \sim v$. Ordinarily authors use n to designate the cardinality of $\mathcal{V}$ and m to designate the cardinality of $\mathcal{E}$. Edges can be undirected, in which case the pairs of vertices are unordered, or they can be directed, in which case one vertex of an edge $\overrightarrow{e}$ is regarded as the *source* and designated $s(\overrightarrow{e})$ and the other as the *target* $t(\overrightarrow{e})$. (When there is a need to distinguish the direction of an edge, arrows will be used to designate directed edges, as in $\overrightarrow{e} \in \overrightarrow{\mathcal{E}}$. The edge from vertex u to vertex v will be designated $\overrightarrow{uv}$, and we shall denote $-\overrightarrow{uv} := \overrightarrow{vu}$. Most often, the focus will be on undirected graphs. In this case, whenever there exists an edge between u and v, for accounting purposes we can consider that the directed edge set includes both $\overrightarrow{uv}$ and $\overrightarrow{vu}$. This is useful because sometimes it will be convenient to introduce an orientation to the edges that occur in a formula, even for undirected edges. Conventions vary, however, so the reader may encounter some discrepancies of factors of 2 when comparing different treatments.

Various levels of complexity can be admitted in graph theory, but to keep things focused, unless explicitly stated otherwise it will be assumed that combinatorial graphs are

- Finite. $m, n < \infty$.
- Connected. Any two vertices can be joined by following a finite sequences of edges.
- Undirected (as described above). However, in some calculations it is convenient to introduce directions on edges.
- Loop-free. We do not consider graphs where there is an edge joining a vertex to itself.
- Unweighted. There is complete democracy among edges!

We can account for how the graph is put together in a number of closely related ways:

- The *adjacency matrix* A
- The *incidence matrix* B
- The *discrete gradient* d and its dual the *discrete divergence* d^*.

The *adjacency matrix* A_{uv} for an undirected graph is 1 when $u \sim v$ and 0 when $u \not\sim v$. The set of $n \times n$ symmetric adjacency martices is in one-to-one correspondence with the set of possible graphs on n vertices, so in a sense all of graph theory can be viewed as the part of linear algebra dealing with matrices of this special form, with various generalizations. The sum of the v-th row or column of the adjacency matrix gives the number of edges connecting to v, known as the $v$alence, or $d$egree of v. Sometimes it will be convenient to organize the degrees into a diagonal matrix with $\mathrm{Deg}_{vv} = d_v$.

Analysis and geometry on graphs relate to two function spaces living on the vertices and, respectively, on the edges, $\mathcal{H}_\mathcal{V}$ and $\mathcal{H}_\mathcal{E}$. When the edges are directed, by convention $\mathcal{H}_{\overrightarrow{E}}$ will be restricted to the set of functions such that $g(-\overrightarrow{e}) = -g(\overrightarrow{e})$.

The *incidence matrix* B identifies which vertices attach to a given edge. It is thus an $n \times m$ matrix where the identification of the column corresponds to an edge and a given row corresponds to a vertex. The ve entry is 1 if edge e is incident to vertex v and otherwise 0.

When used an an operator, the incidence matrix relates the space of functions on the edges to the space of functions on the vertices. These spaces are isomorphic to finite-dimensional vector spaces when the graph is finite: $\mathcal{H}_\mathcal{V} = \mathbb{C}^n$ and $\mathcal{H}_\mathcal{E} = \mathbb{C}^m$. Both spaces are inner-product spaces with

$$\langle f_1, f_2 \rangle_\mathcal{V} := \sum_{v \in \mathcal{V}} f_1(v)\overline{f_2(v)},$$

$$\langle g_1, g_2 \rangle_\mathcal{E} := \sum_{e \in \mathcal{E}} g_1(e)\overline{g_2(e)}. \tag{8}$$

The function space for undirected edges is isomorphic to an m-dimensional subspace of $\mathcal{H}_{\overrightarrow{\mathcal{E}}}$, for which

$$\langle g_1, g_2 \rangle_{\overrightarrow{\mathcal{E}}} := \sum_{\overrightarrow{e} \in \overrightarrow{\mathcal{E}}} g_1(\overrightarrow{e})\overline{g_2(\overrightarrow{e})}.$$

In analysis on Euclidean spaces the gradient acts on functions and to each vector in the tangent space at a given point it assigns a value. The closest thing on a discrete graph to the tangent space at a point of a manifold is

the set of directed edges. Correspondingly, in the setting of a graph we can define a gradient operator $d : \mathcal{H}_{\mathcal{V}} \to \mathcal{H}_{\overrightarrow{\mathcal{E}}}$ via

$$[df](\overrightarrow{e}) = f(t(\overrightarrow{e}) - f(s(\overrightarrow{e})).$$

There is a dual operator analogous to the divergence in vector analysis, *viz.*, $d^* : \mathcal{H}_{\overrightarrow{\mathcal{E}}} \to \mathcal{H}_{\mathcal{V}}$ such that

$$[d^*g](v) = -2 \sum_{\overrightarrow{e}: v = s(\overrightarrow{e})} g(\overrightarrow{e}).$$

With the convention that the directed edge set for an undirected graph includes both orientations of an (undirected) edge e, we calculate

$$\langle df, g\rangle_{\overrightarrow{\mathcal{E}}} = \langle f, d^*g\rangle_{\mathcal{V}}\,.$$

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

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

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

2.1. **Other operators on graphs.** The adjacency matrix and the standard graph Laplacian as defined above are self-adjoint matrices that reflect the structure of a graph through their eigenvalues and eigenvectors, and they have been extensively studied for this purpose. See, for instance, [11, 15, 21] for this subject, especially as regards the graph Laplacian and the adjacency matrix.

There are many additional operators that naturally live on a graph. For example, there is the signless Laplacian,

$$Q := \mathrm{Deg} + A = BB^*. \tag{9}$$

Some authors, especially Chung [14], prefer a normalization for the Laplacian by which the diagonal elements are all 1. This can be achieved by weighting the Hilbert space $\mathbb{C}^n$ proportionally to the degree of a given vertex. Equivalently, we can define the renormalized Laplacian as

$$\mathcal{L} := \mathrm{Deg}^{-1/2}\, L\, \mathrm{Deg}^{-1/2}\, D = I - \mathrm{Deg}^{-1/2}\, A\, \mathrm{Deg}^{-1/2}\,. \tag{10}$$

The operators A, L, Q, and $\mathcal{L}$ 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, and their eigenvalues relate in somewhat different ways to the features of the graph.

A Schrödinger operator on a combinatorial graph can be defined as $L+V$, where V is a diagonal matrix on the vertex space, called the "potential energy." Some physicists study these as discrete models of quantum systems, for example in the Anderson model, where the potential energy may be generated by a random process. Because the degree matrix is diagonal, it is often absorbed into V when studying Schrödinger operator on graph. When we consider quantum graphs below, a potential energy will reside on the edges rther than the vertices. (Though there is no real barrier to considering potential energies on the edges of a quantum graph as well.)

A diagonal potential energy corresponds to what physicists term a *scalar* interaction, but vectorial interactions are also important in physics, especially in connection with magnetism. If we discretize a magnetic Schrödinger operator the effect of the field shows up by causing phase factors to appear in the wave function when an edge is traversed. One approach to defining magnetic operators on graphs is to begin with a quadratic form such as

$$E_\theta(f) := \sum_e |f(te) - e^{i\theta(e)} f(se)|^2. \tag{11}$$

Weights could also be included. When the graph is unbounded, it is essential to consider conditions that will guarantee that either a scalar or magnetic Schrödinger operators are well-defined and self-adjoint. We refer to the work of Colin de Verdière and Torki [18, 19] for questions of self-adjointness when the graph is unbounded. For work on spectral analysis of magnetic Laplacians, see also [15, 38, 22].

Analogues of other important differential operators, notably Dirac operators, may also be defined on graphs, as is discussed in the course of Golénia at this workshop.

3. Can one hear the shape of a graph?

Following the classic query of Kac from 50 years ago, "Can one hear the shape of a drum?" characterizing curiosity about how much information is contained in the eigenvalues of the problem of a vibrating membrane, we can ask: Given the eigenvalues of one or other of the matrices described in the preceding section, can we determine the structure of a graph? Of course we have utterly no interest in how the graph is placed in space,

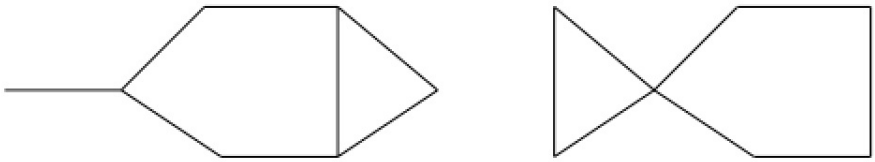

FIGURE 1. Mouse and Fish

and in particular we don't distinguish between graphs where we have just relabeled the vertices by a permutation.

By the spectral diagonalization of matrices, a graph certainly is determined by the eigenvalues along with a basis of eigenvectors. The more subtle question is whether there is enough information in the set of eigenvalues of one of the operators A, L, Q, etc. to recover A up to a permutation, without knowledge of the eigenvectors. Note that there are only finitely many possible $n \times n$ distinct adjacency matrices: $\frac{2^{n(n-1)/2}}{n!}$ of them, if we account for permutations. Meanwhile, there is no obvious way to characterize which values are possible for a given eigenvalue, say the 3rd one, and which are not. But why not conjecture at least that the eigenvalues determine the graph in principle?

It turns out that there are simple examples of *cospectral* graphs, which are not isomorphic, yet have precisely the same eigenvalues. For the case of the graph Laplacian, one such pair, which I call "mouse" and "fish," is shown in Figure 1. Other simple examples are known for the adjacency matrix, the renormalized Laplacian, etc.

Contemplating mouse and fish, we immediately see that the degrees of the vertices are not determined by the spectrum, and since the set of degrees is one of the most basic properties of a graph, this is disappointing. On the other hand, we see that some features of the two graphs are the same, including the number of vertices, the number of edges, and the number of trianges, and indeed, all of these can be determined almost immediately from the eigenvalues of one or other of the graph's matrices, as we shall soon see.

After the article by Kac, people sometimes refer to a feature of an operator that can be determined from its eigenvalue spectrum as *audible*, or say that it can be *heard*. In life, things can be heard clearly, or indistinctly, and the same is true of features of a graph; perhaps we cannot determine a

feature exactly, but the eigenvalues might be used to find a bound on the size of that feature, or a relationship to other features.

As we shall see, the information contained in the eigenvalue spectrum of each of the standard operators is a little different from the others. So, in addition to determining whether a feature is audible, we may ask, "with which ear?"

In the theory of Sturm-Liouville equations, it has been known since the work of Gel'fand and Levitan [30] that it typically suffices to have two independent spectra, for instance one with a Dirichlet condition at an end point and another with a Neumann condition there, to uniquely determine the details of the operator from the spectrum. It would be reasonable to hope for a similar uniqueness theorem for graphs, but I am unaware of a satisfying theorem of this nature.

Another typical feature of inverse spectral problems is that whereas the problem is not well-posed in general, it is nonetheless the case that the spectrum sometimes does uniquely determine the operator, especially when some aspect of the spectrum is maximized or minimized. Again, there do not appear to be many results of this type for operators on graphs.

Data analysis and questions of computational complexity often focus to locating or quantifying features like the following subsets and properties.

(1) *Clusters*, or *communities*. Which parts of a graph are much more closely connected within themselves than to the rest of the graph? As a first step to this is the question of how to define a cluster in a quantitative way, and the literature (e.g., [2]) in fact contains various alternatives.
(2) *Cliques*, which are induced subgraphs that are complete. (An *induced* subgraph of G is the part of the graph containing a certain subset of the vertices and all edges in G that connect vertices in the subset. *Complete* means that a graph or subgraph is maximally connected.)
(3) Quasi-stable subsets. If we set up a diffusive process on the graph, there may be regions where the density diminishes rapidly, and otheres where it is nearly in equilibrium. Intuitively, these regions may resemble the clusters mentioned above, but they are defined dynamically. The lectures by Anantharaman address related ideas.
(4) *Colorings*. How many colors are minimally necessary to assign to the vertices, so that no edges connect two vertices of the same color? (This is known as the *chromatic number* of the graph.) What are the

subsets of a given color? As an alternative, edges could be colored with the analogous rule.

(5) How easily is a graph disconnected? I.e., how many edges must be removed so that it is no longer a connected set?

(6) *Spanning trees.* A *tree* is a graph that has no closed cycles, so a general graph can be reduced to a tree that includes all of the same vertices simply by removing enough edges. Such spannng trees are important in computation, because efficient algorithms, such as Dijkstra's algorithm, proceed by constructing them.

In these notes we will not be able to do more than touch on some of the simplest known facts about the aspects of a graph which are audible through the eigenvalies of its associated operators. In this regard we shall be mostly concerned with the graph Laplacian L.

The operator L has a special relation to the vector all of whose entries are the same. Let $\mathbf{1}$ denote the vector of "all ones." It is immediate that $L\mathbf{1} = \mathbf{0}$, but is $\mathbf{1}$ the only vector in the null space (up to multiples)? Already from the weak form

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

we can easily see that the dimension of the null space is the number of connected components, because $E(f) = 0$ forces the vector to be constant on any component, but makes no restriction connecting the values on different components. The dimension of the null space is synonymous with the multiplicity of the eigenvalue 0, so, trivially, the number of connected components of a graph is audible. (As remarked above, for the most part we shall restrict our attention to connected graphs, other than to call attention to this fact.)

Another feature of the graph that is trivially audible is the number n of vertices, provided that it is finite, since it is simply the number of eigenvalues, counting multiplicities. Here it is irrelevant which operator associated to the graph we regard, since all of the choices we consider are $n \times n$ symmetric matrices. Slightly less obvious is that the number m of edges is audible. This is because the sum of the degrees is equal to $2m$, since d_v counts the number of edges incident to v, but when we sum over all the vertices, each edge is accounted for exactly twice, once for each endpoint. Since the diagonal part of L consists of the numbers d_v, we have

$$\mathrm{tr}(L) = \sum_j \lambda_j = \sum_v d_v = 2m.$$

The edge count m is also easily determined from the eigenvalues of A by the following argument. What is the meaning of the uv-component of A^k? Reflecting on this, it is clear that it counts the number of ways that one can pass from vertex u to vertex v in k steps. In particular, $A^2_{vv} = d_v$ and $A^3_{vv} = 2t_v$, where t_v denotes the number of triangles in G of which v is a vertex. (Each triangle is counted once clockwise and once counterclockwise.) By taking the trace of A^2 and of A^3 we can thus determine the total number of edges and triangles in a graph from the sum of the squares and, respectively, cubes, of the eigenvalues of A. The number if triangles is thus audible in terms of the adjacency spectrum, per the formula $T(G) = \frac{1}{6} \operatorname{tr} A^3$.

Is it just as easy to count other cycles, like squares, pentagons, and so forth? Certainly we can approach these questions with traces of powers of A, although intricate combinatorial and number-theoretic 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.

Similar information can be obtained form the traces of powers of L, but entangled with some other information, such as the Zagreb index

$$Z_G := \sum_v d_v^2,$$

which is a topological index related to the statistical distribution of degrees, since the standard deviation of the numbers d_v is expressible in terms of Z and m. We calculate for instance

$$\operatorname{tr}(L^2) = \operatorname{tr}(\operatorname{Deg}^2 + A^2 - A \operatorname{Deg} - \operatorname{Deg} A) = Z_G + 2m,$$

and even

$$\begin{aligned} \operatorname{tr}(L^3) &= \operatorname{tr}(\operatorname{Deg}^3 - A \operatorname{Deg}^2 - \operatorname{Deg}^2 A - \operatorname{Deg} A \operatorname{Deg} \\ &\qquad + A^2 \operatorname{Deg} + A \operatorname{Deg} A + \operatorname{Deg} A^2 - A^3) \\ &= 4\Sigma d_i^3 - 6T, \end{aligned} \tag{12}$$

where Σd_i^3 is again related to the statistical skewness of the distribution of degrees.

From these formulae it is not clear that the number of triangles is audible in the spectrum of L, without knowing something about the statistics of the degrees. Indeed, there is an example of a pair of Laplacian-cospectral graphs with $n = 6$, one of which has a triangle while the other does not. (See [11], §14.4.1.)

As to spanning trees, a classic theorem of Kirchhoff states that the number of spanning trees of a graph is equal to the product of the non-zero eigenvalues of the graph Laplacian, divided by n [10, 23]. Hence the number of spanning trees is audible in th spectru of L.

It is not generally possible to solve for the eigenvalues of an $n \times n$ matrix like L or A in closed form, but there are efficient ways to compute them. Some ways of approximating eigenvalues "variationally" are useful for proving theorems as well as for making calculations.

The spectral theorem, as discussed in Najar's lectures or in texts such as [1, 40, 44], is at the heart of variational characterizations of eigenvalues. One of its useful consequences is the following.

Theorem 1. *Suppose that $H = H^*$ on some Hilbert space. 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.

Proof. The definition of an approximate eigenvector includes the possibility that λ might be a true eigenvalue. In that case the statement of the theorem follows by taking each φ_k to equal the normalized eigenvector.

Otherwise, suppose that for some λ, $(H-\lambda)\varphi_k \to 0$, but that $(H-\lambda)\varphi_k =: \zeta_k \neq 0$. It follows that

$$\frac{\|(H-\lambda)^{-1}\zeta_n\|}{\|\zeta_n\|} = \frac{1}{\|(H-\lambda)\varphi_k\|} \nearrow \infty.$$

Therefore $(H-\lambda)^{-1}$ cannot be a bounded operator, and hence $\lambda \in \sigma(H)$.

Conversely, if $\lambda \in \sigma(H)$, then $\chi_{(\lambda-1/k,\lambda+1/k)}(H) \neq 0$, where we use the spectral theorem to define $\chi_{(\lambda-1/k,\lambda+1/k)}(H)$ as an orthogonal projector. Since this projector is not the zero operator, there exists $\phi_k \in \mathrm{Ran}\chi_{[\lambda-1/k,\lambda+1/k]}$, $\|\phi_k\| = 1$, and we again appeal to the spectral theorem to conclude that

$$\|(H-\lambda)\varphi_k\|^2 = \int_{\lambda-\frac{1}{k}}^{\lambda+\frac{1}{k}} (x-\lambda)^2 d\mu_{\phi_k} < \frac{2}{k} \to 0.$$

□

It is sometimes useful to quantify how close one of the approximations of this kind comes to being a true eigenvector. The spectral theorem can be used to provide estimates like the following.

Exercises.

(1) Suppose that λ is an isolated eigenvalue (possibly non-simple) of H and $\psi \in \mathcal{D}(H)$, $\|\psi\| = 1$. Let $\delta := \mathrm{dist}(\lambda, sp(H)\backslash\lambda)$, and let P be

the spectral projector for λ. If the *residual* $\|(H-\lambda)\psi\| \le \delta' < \delta$, then

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

(2) Generalize the lemma of Exercise 1 to the case where there is a narrow cluster of eigenvalues isolated from the rest of the spectrum by distance δ.

One of the most important tools for estimating spectra of a self-adjoint operator or matrix is the min-max principle (e.g., [3]). The reader is warned that numbering conventions for eigenvalues are not universal, with some sources preferring to number them in increasing order and others in decreasing order. To avoid confusion over this small point, eigenvalues will sometimes be equipped with arrows to indicate which way they are ordered.

Theorem 2. *Let H be an operator on a Hilbert space $\mathfrak{H}$, and suppose that $H = H^* \ge CI$ for some $C > -\infty$ and that there are N eigenvalues $\lambda_1^\uparrow \le \lambda_2^\uparrow \le \cdots \le \lambda_N^\uparrow$ below the essential spectrum of H. For any $\mathfrak{M} \subset D(H)$, define $\lambda(\mathfrak{M}) := \sup\langle H\varphi, \varphi\rangle : \varphi \in \mathfrak{M},\ \|\varphi\| = 1$. Set*

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

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

To clarify terms, the *essential spectrum* consists of the accumulation points of the spectrum and the eigenvalues with infinitely many independent eigenvectors, and $D(H)$ is the domain of definition of H, which is not necessarily all of $\mathfrak{H}$. For finite-dimensional matrices, like those we associate with a finite graph, these qualifiers are not needed, since there is no essential spectrum, and $D(H)$ is the entire space on which the matrices act.

Furthermore, if H is a finite matrix, then we can apply min-max to $-H$, and get a max-min characterization of the eigenvalues counting from the top.

Here is a sketch of the proof of the min-max principle.

Proof. It is clear from the definition that $\tilde{\lambda}_\ell^\uparrow \le \lambda_\ell^\uparrow$, so we show the inequality in the other direction. Given the orthonormalized eigenvectors $\{\psi_j\}$, let

$$M_\ell := \text{span } [\psi_1 \cdots \psi_\ell],$$

and let P be the orthogonal projector onto $M_{\ell-1}$. Since the dimension of $M = \ell$ exceeds that of $M_{\ell-1}$, there exists $f \in M \perp \text{Ran}P$ with $\|f\| = 1$. Then

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

which establishes that $\tilde{\lambda}_\ell^{\uparrow} \geq \lambda_\ell^{\uparrow}$. □

Credit for the discovery of the min-max principle is uncertain, with related results and variants often attributed to Rayleigh, Ritz, Courant, Fischer, and Weyl. When $\ell = 1$ the min-max principle is known as the *Rayleigh-Ritz inequality*, which states that for all $\varphi \in D(H)$, $\varphi \neq \mathbf{0}$,

$$\lambda_1^{\uparrow} \leq \frac{\langle H\varphi, \varphi\rangle}{\|\varphi\|^2}. \tag{13}$$

A variant of Theorem 2 is often preferred in practice because the way the test spaces are defined is more computationally convenient, *viz.*,

Theorem 3. *Under the same assumptions, For any $\mathfrak{M} \subset \mathfrak{H}$, define $\mu(\mathfrak{M}) := \inf\langle H\varphi, \varphi\rangle : \varphi \in D(H), \varphi \perp \mathfrak{M}$, $\|\varphi\| = 1$. Set*

$$\tilde{\mu}_\ell^{\uparrow} := \sup\{\mu(\mathfrak{M}) : \mathit{dim}(\mathfrak{M}) = \ell - 1\}$$

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

Among the corollaries of the min-max principle is the *Courant-Weyl* theorem, which is given as the following somewhat challenging Exercise (1) (or see [11] or [21], but be aware that the eigenvalues are decreasingly ordered there):

Exercises.

(1) Prove that if A and B are self-adjoint matrices, then

$$\lambda_k^{\uparrow}(A) + \lambda_1^{\uparrow}(B) \leq \lambda_k^{\uparrow}(A+B) \leq \lambda_{k+1}^{\uparrow}(A) + \lambda_{n-1}^{\uparrow}(B). \tag{14}$$

The Courant-Weyl formula (14) also holds for self-adjoint operators A and B subject to having discrete spectrum and some technical conditions.

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

(3) Under the same circumstances as in the min-max principle, suppose that $\{\phi_1, \ldots, \phi_\ell\}$ is an orthonormal set of functions in the quadratic-form domain of H. Prove the *variational principle for sums*,

$$\sum_{j=1}^{\ell} \lambda_j^{\uparrow} \leq \sum_{j=1}^{\ell} E_H(\phi_j), \tag{15}$$

cf. [3], ch. 2, §34.

4. Graph Laplacians and their spectra

Some simple graphs have eigenvalues and eigenvectors that are easy to find, and we shall find that they are useful aids to understand the spectra of more complicated graphs. For example, the complete graph on n vertices has a graph Laplacian of the form $n(\mathbb{I} - P_{\mathbf{1}})$, where $P_{\mathbf{1}}$ is the projector onto the vector 1. For example, with $n = 7$,

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

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

As with all graph Laplacians, $L_{K_n}\mathbf{1} = \mathbf{0}$. We also see that for any $f \perp \mathbf{1}$, $L_{K_n} f = nf$. Thus every vector with components having mean 0 is an eigenvector with the eigenvalue n. Because of this, we shall follow a numbering convention for the eigenvalues beginning with 0, so that, assuming that G is connected, $0 = \lambda_0 < \lambda_1 \leq \ldots \lambda_{n-1}$. Although this convention may seem to be inconsistent with that of the min-max principle 2, it becomes the same if consider the graph Laplacian as acting on the Hilbert space of n-component vectors orthogonal to $\mathbf{1}$.

An extreme case is when $n = 2$, for which K_2 is the only connected possibility. It has eigenvalues 0 and 2. The *edge Laplacians* L_e for an edge e can be used to build up an arbitrary graph G by

$$L_G = \sum_{e \in \mathcal{E}(G)} L_e. \tag{16}$$

(More carefully, L_e should be written $L_e \oplus 0$, where the 0 operator operates on the complement in G of e, but we shall abuse notation and use L_e also to denote the graph on n vertices, containing only the edge e.) One immediate consequence of this and the observation that $L_e \geq 0$ in the sense of matrices is that:

If an edge is appended to a graph, then each eigenvalue of the graph Laplacian either stays the same or increases.

Verification Exercise. Use the min-max principle to prove this fact formally.

In particular, the eigenvalues of L_{K_n} are maximal among all graph Laplacians on n vertices. All eigenvalues of any graph Laplacian lie in the interval $[0, n]$.

The *complementary graph* G^c to a graph G has edges connecting the pairs of vertices that are not connected in G, and vice versa. The adjacency matrices differ off the diagonal by $0 \leftrightarrow 1$. For example,

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

and

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

are adjacency matrices of the complementary graphs depicted in Figure 2. If we include the union of the edges of a graph and its complement, we get the complete graph K_n. That is, $A_G + A_{G^c} = A_{K_n}$, and consequently

$$L_G + L_{G^c} = L_{K_n} = n(\mathbb{I} - P_{\mathbf{1}})$$

This formula implies a close relationship between the spectra of G and G^c:

Proposition 1. *The nonzero eigenvalues of L_G and L_{G^c} are related by*

$$\lambda \in sp(L_G) \Leftrightarrow n - \lambda \in sp(L_G^c),$$

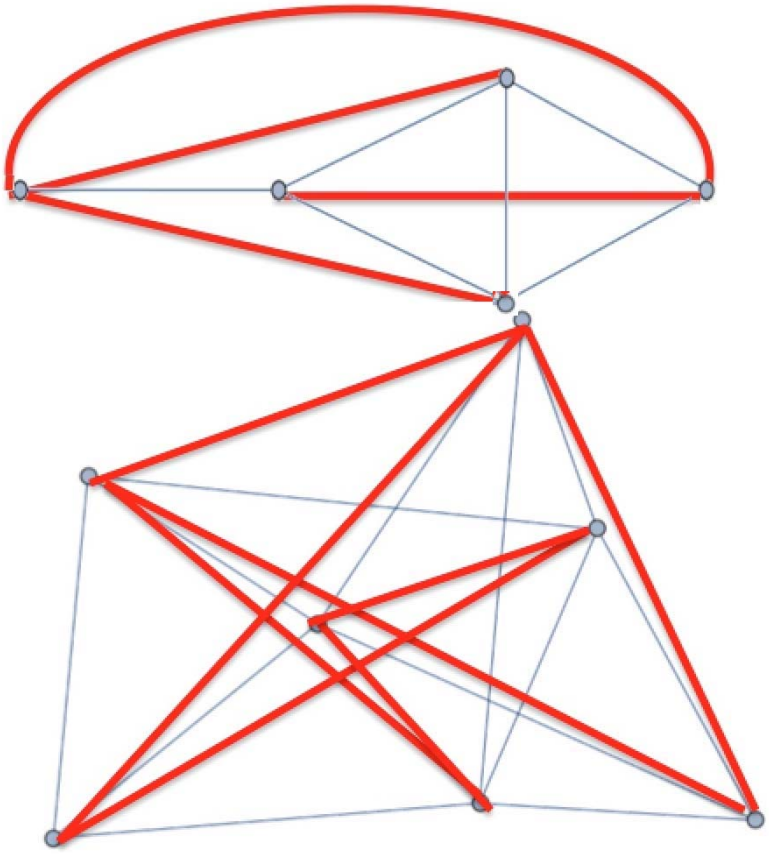

FIGURE 2. Complementary pairs of graphs

and they have the same eigenvectors.

Let us next ask about graph colorings, the subject of the famous four-color map theorem for planar graphs. How many colors are needed so that each vertex in G can be assigned a color, such that no adjacent vertices have the same color? The minimal number of necessary colors is called the graph's chromatic number, $\chi(G)$. Is $\chi(G)$ audible? Are there at least spectral methods that give some indications about it? We shall see that it is efficient to use eigenvalues to determine whether a graph is two-colorable, or *bipartite*, which is an important category of graphs in many applications. It is not difficult to prove that a graph is bipartite iff it contains no closed paths of odd length.

Efficiently determining when a graph G has $\chi(G) = 3$, however, is a major open problem, with implications for the study of algorithms (e.g., [13]).

Here is a simple theorem showing that $\chi(G) = 2$ is audible in terms of the normalized or signless Laplacian.

Theorem 4. *A connected finite graph with more than one vertex is bipartite iff either of the following is true.*

(1) 0 *is an eigenvalue of the signless Laplacian* Q.
(2) 2 *is an eigenvalue of the renormalized Laplacian* $\mathcal{L}$.

Proof. If $\mathcal{L} = I - \mathrm{Deg}^{-1/2} A \,\mathrm{Deg}^{-1/2}$ has eigenvalue 2, then, multiplying by $\mathrm{Deg}^{1/2}$ and rearranging,

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

for some nonzero w. Leting $u := \mathrm{Deg}^{-1/2} w$, this reads $Qu = 0$. The two conditions are thus equivalent, since the argument just given is reversible.

Recalling now 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 connected vertices $u \sim v$. The sign of f_v gives a 2-coloring of the vertices of G, provided that G is connected. □

We note that without connectedness the eigenfunction could simply vanish on one of its components, invalidating the proof. Indeed, the star graph on 4 vertices and the disjoint union of a triangle K_3 and an isolated point are Q-cospectral, but only the former is bipartite. (Example from [11].)

In contrast, the Laplacian is "deaf" to whether a graph is bipartite, due to the example found in [11] mentioned earlier, of a Laplacian-cospectral pair, one of which is bipartite graph, while the other contains a triangle.

Exercise. Show that a connected graph G is bipartite if and only if the lowest and highest eigenvalues of A satisfy $\alpha_{\min} = -\alpha_{\max}$.

The Courant-Weyl formula (14) allows us to understand the effect of changing the graph in some simple ways. For example, if we append an edge to a graph, with the aid of (14) we can derive an *interlacing theorem* from the edge-decomposition formula (16):

Theorem 5. *Let $G + e$ designate the graph G on n vertices with the edge e appended, with $e \notin \mathcal{E}(G)$. Then the eigenvalues of the Laplacians of the*

two graphs satisfy

$$\lambda_k^{\uparrow}(L_G) \leq \lambda_k^{\uparrow}(L_{G+e}) \leq \lambda_{k+1}^{\uparrow}(L_G).$$

Proof. The first inequality follows from the min-max principle, since $L_{G+e} = L_G + L_e \geq L_G$. For the second inequality in the theorem, we use the second inequality in (14), choosing A as L_G and B as L_e, considered as an operator on the whole vertex space. Because L_e has rank 1, its null space has rank $n-1$, implying that $\lambda_{n-1}^{\uparrow}(L_e) = 0$, proving the claim. □

4.1. **Hunting for eigenvalues with variational weapons.** To this point we have used special properties of the matrices L, A, etc. to learn about the graph from the spectrum, but now we ask what can be learned from general "variational methods," based on min-max, Courant-Weyl, the variational principle for sums, etc. These are standard tools in numerical analysis to "hunt" for eigenvalues, in the sense of determining where they are on the number line, but for our purposes the goal will be more to relate their distribution to properties of the graph.

One of the simplest uses of the variational principle for sums (15) reveals something about the distribution of the degrees of the vertices of a graph:

Theorem 6. *The sum of the lowest k eigenvalues of L is bounded above by the sum of the lowest k degrees d_v.*

Proof. Since the degrees are on the diagonal of L, $d_v = \langle L\mathbf{e}_v, \mathbf{e}_v\rangle$, where $\mathbf{e}_v$ is the standard unit vector equaling 1 on the vertex v and 0 everywhere else. We apply (15) choosing $\phi_j = \mathbf{e}_{v_j}$, where v_j, $j = 1, \ldots \ell$ are the vertices with the largest ℓ degrees. □

One good strategy to hunt for eigenvalues of a generic graph G is to use as trial functions the eigenvectors of some special graphs where the analysis is explicit. An example of such a special graph is the complete graph K_n. As pointed out above, every vector orthogonal to $\mathbf{1}$ is an eigenvbector with eigenvalue n. One might be inclined to create an orthonormal set of $n-1$ of these by using the Gram-Schmidt procedure, but this isn't really necessary. In fact one of the simplest ways to organize the eigenspace is to use a "superbasis" of functions supported on individual edges $h_{u\vec{v}} = \mathbf{e}_u - \mathbf{e}_v$., i.e.,

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

The number of such trial functions is $n(n-1)$, far larger than a basis, but this set has a similar distinction of being a *tight frame*, which means that that it enjoys a sort of completeness relation but with a multiple other than 1. In particular, a calculation shows that for vectors f of mean 0 (i.e., $\perp \mathbf{1}$):

$$\begin{aligned}\sum_{e\in\vec{\mathcal{E}}} |\langle h_e, f\rangle|^2 &= \sum_{u,v} |f_u - f_v|^2 \\ &= \sum_{u,v} (|f_u|^2 + |f_v|^2) - 2Re \sum_{u,v} f_u \overline{f_v} \\ &= 2n \sum_w |f_w|^2 - 0 \\ &= 2n\|f\|^2. \end{aligned} \tag{17}$$

(Since the constant vector $\mathbf{1}$ is automatically in the null space of L, we can effectively consider that L is an operator on the Hilbert space of vectors $\perp \mathbf{1}$. It is the latter on which the vectors h_e constitute a tight frame.)

While the variational principle for sums (15) requires an orthonormal set of test functions, there is an equivalent theorem which does not require orthogonalization, but instead requires an average of expressions of the form $E(\phi)$. The *averaged variational principle* is particularly suited for the situation when the test functions are a subset of a tight frame:

Theorem 7. [33] *Let Q_M be a self-adjoint quadratic form on a Hilbert space $\mathfrak{H}$ with purely discrete spectrum consisting of eigenvalues that are ordered (counting multiplicities), so that*

$$-\infty < \mu_0 \leq \mu_1 \leq \dots .$$

Let $\mathfrak{M}$ be a measure space indexing a tight frame of vectors such that for any $\phi \in \mathfrak{H}$,

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

for some fixed $A > 0$. Let $\mathfrak{M}_0 \subset \mathfrak{M}$ be any subset such that $|\mathfrak{M}_0| > kA$. Then

$$\frac{1}{k}\sum_{j=0}^{k-1} \mu_j \leq \frac{1}{|\mathfrak{M}_0|} \int_{\mathfrak{M}_0} \frac{Q_M(f_\zeta, f_\zeta)}{\|f_\zeta\|^2} d\sigma. \tag{18}$$

To bring this down to earth, in the case of a self-adjoint matrix M, $Q_M(\phi,\phi)$ means $\langle M\phi, \phi\rangle$, and the condition on the eigenvalues is automatic.

We now see what happens when we use the vectors h_{uv} in the averaged variational principle. The measure is just the counting measure, so the integrals are sums. We calculate:

$$Lh_{uv}(w) = d_u\delta_u - d_v\delta_v + \vec{A}_{\cdot v} - \vec{A}_{\cdot u}, \tag{19}$$

where

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

and $\vec{A}_{\cdot v}$ is the column vector of the adjacency matrix in the v position. We thus get

$$\langle Lh_{\vec{uv}}, h_{\vec{uv}} \rangle = d + u + d_v + 2a_{uv}. \tag{20}$$

Verification Exercise. Confirm (19) and (20) by considering the different possibilities separately, whether $w = u$ or v, $w \sim u$ or v, or $w \not\sim u$ or v.

From the averaged variational principle (multiplying through by k we can make a quantitative statement showing that large sums of eigenvalues require a high degree of connectedness:

Corollary 1. *([33]) Let G be a finite connected graph on n vertices. Then for $1 \leq k < n-1$, the eigenvalues $0 = \lambda_0 \leq \lambda_1 \leq \cdots \lambda_{n-1}$,*

$$\sum_{j \leq k} \lambda_j \leq \frac{1}{2n} \min_{\textit{choices of } nk \textit{ pairs}} \sum_{uv} (d_u + d_v + 2a_{uv}).$$

Exercise. For the normalized graph Laplacian, numbering the eigenvalues $\mathfrak{c}_j$ as in the previous corollary, show that

$$\sum_{j=1}^{k} \mathfrak{c}_j \leq \frac{1}{4m} \min_{\text{choices of } nk \text{ pairs}} \sum_{uv} (d_u + d_v + 2a_{uv}),$$

cf. [33].

We also note the following results for the adjacency matrix and its square:

Exercise. Let G be a finite connected graph on n vertices. Show that for $1 \leq k < n-1$, the eigenvalues $\alpha_0 \geq \alpha_1 \geq \cdots \alpha_{n-1}$ of the adjacency matrix

A_G satisfy the elementary inequalities

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

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

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

cf. [33].

There is far more to learn about the subject of operators on combinatorial graphs, known as "algebraic graph theory," and about their spectra, and the curious reader is invited to look at sources such as [8, 11, 14, 15, 21]. In the next section we shall bring the edges to life, but before leaving combinatorial graphs, let us list some open challenges for the future.

(1) The essential open problem in spectral graph theory is to find spectral conditions to determine a graph uniquely (up to permutations) Are there two independent spectra that accomplish this? Since the standard operators A, L, Q, and $\mathcal{L}$ are equivalent for regular graphs, some truly distinct other operator needs to be brought into the game. Could it be one of these with an additional "boundary condition" imposed?
(2) How many different graph spectra are there, for instance for the Laplacian on n vertices, and what universal constraints characterize the possible spectra?
(3) To what extent it the inverse spectral problem localizable for graphs? Consider that the vectors h_e are eigenvectors not just for a complete graph, but for any graph that contains a clique $\mathcal{C}_\infty$ that lies within a larger clique $\mathcal{C}_\in$ such that no edges connect $\mathcal{C}_\infty$ to the vertices outside $\mathcal{C}_\in$, so at least this feature can be tested for locally. What other features of subsets of a graph can be tested for variationally?

5. Quantum graphs

In this section we allow the edges to be intervals, on which something interesting happens, wich certainly would include a differential equation! There are many reasons to do this, connected to modeling of phenomena that take place on networks, where some sort of physical process on the connections of a network interact with the vertices at its ends. A network of infinitesimally thin channels, known as *quantum wires*, is such a model. Imagine a waveguide where the width of the channel is of nanoscale while the lengths are macroscopic. Physically, one would expect that a one-dimensional model would be a decent approximation, but any limit used to make this connection is singular and involves mathematical subtleties, especially at the vertices. We refer to [9, 26, 27, 39], which contain some discussion of modeling that leads to quantum graphs, among other things.

There are many ways in which one-dimensional models relying on differential equations can operate on the edges of a *metric graph*, in which the edges have the topology of intervals, but I shall discuss only Schrödinger equations:

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

and will be largely guided by the monograph by Berkolaiko and Kuchment [6] and by Berkolaiko's introductory treatment [4], which go far beyond these lectures and are recommended to the interested student. Often, the potential energy $V(x)$ will be set to zero, and since we do not consider potential energy at the vertices, this would define a Laplacian.

As to the structure of the underlying metric graph, edge lengths will be allowed to vary, and even to be infinite. Loops are also allowed. For technical reasons we assume that every edge has length $\geq \delta$ for some fixed $\delta > 0$. An important concern is how the edges are connected at vertices. What conditions do we impose there, so that the quantum graph is something more interesting than a collection of independent intervals?

Again, there are many choices as categorized in [6], but here we shall always choose "Kirchhoff" or "Neumann-Kirchhoff" conditions,

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

which are mathematically the simplest from many points of view.

Since we have abandoned discreteness, it will be necessary to consider some questions of analysis that did not arise earlier. For spectral theory, linear differential operators are usually defined with reference to Sobolev spaces.

The *Sobolev space* H^1 on a metric graph G is defined by completing the continuous, compactly supported functions in the Sobolev norm for the orthogonal sum of Hilbert spaces of the form

$$\oplus_{e\in\mathcal{E}(G)}\, H^1(e, dx_e) \tag{21}$$

where dx_e is the coordinate corresponding to arclength on the edge e. The Sobolev H^1 norm is given by

$$\|f\|^2_{H^1} := \sum_{e\in\mathcal{E}(G)} \int_e (|f'|^2 + |f|^2) dx_e.$$

The condition of continuity specifically includes the requirement of continuity at the vertices, and it is this fact which makes $H^1(G)$ a closed strict subset of (21). Indeed, on intervals functions in H^1 are continuous, including at the end points. (More technically, they are equivalence classes of functions containing representatives that are continuous.) Hence the functions in $H^1(G)$ are continuous at the vertices (up to equivalence classes).

The weak form of a *quantum-graph Hamiltonian* H is given by

$$f \in H^1(G) \to \sum_{e\in\mathcal{E}} \int_e (|f'(x_e)|^2 + V(x)|f(x_e)|^2 dx_e. \tag{22}$$

To avoid some technical issues, we'll always assume that $V(x) \geq C > -\infty$ and continuous. Observe that if $V = 0$, then (22) is precisely the weak form one would choose to define the Laplacian on a metric graph by the Friedrichs extension, following the ideas of §1.

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 $\langle Hf, f\rangle$, using the L^2 inner product on G.

Let's consider some simple examples, especially with reference to their spectra. Note that the eigenvalues of quantum-graph Hamiltonians are bounded from below but not from above, so they will always be given the increasing order, and in this section we will not encumber them with arrows.

(1) A single interval $-1 \leq x \leq 1$ with $V = 0$. However, let's pretend that there is a vertex in the middle! At the end vertices $x = \pm 1$, there is only one incident edge, so the Kirchhoff condition becomes the classical Neumann boundary condition that $f'(\pm 1) = 0$. Meanwhile, for the vertex at 0, the Kirchhoff condition that the sum of the

outgoing derivatives is 0 is the same as saying that the left and right derivatives at 0 are the same, and that just means that the function f is differentiable at 0. When you think about this, on a quantum graph, *having a vertex of degree 2 between edges $e_{1,2}$ is equivalent in every respect to having a single edge continuously joining e_1 and e_2, with no vertex between them.* It is, however, frequently useful in proving theorems to imagine such bogus vertices appearing at convenient positions in the interior of an edge.

To turn now to the spectrum, recall that the eigenvalues and eigenvectors for a single interval of length 2 are determined as follows. With

$$-\psi'' = \lambda\psi$$

and setting $\lambda = k^2$, we find with the Neumann conditions that $k_\ell = \frac{\pi\ell}{2}$ and, up to a normalization constant,

$$\psi(x) = \cos\left(\frac{\pi\ell}{2}(1+x)\right), \ell = 1, 2, \dots.$$

(2) A Y-graph, $V = 0$. By this we mean that three intervals of lengths $L_e < \infty$ are joined at a single vertex. We'll fully treat the case where all $L_e = 1$, leaving details for the case of differing L_e as an exercise. Because the isolated end points of the edges have Neumann boundary conditions, we know that the eigenfunctions are proportional to $\psi_e(x_e) = \cos(k(1-x_e))$, where the edge variables x_e increase from the value $x_e = 0$ at the vertex that joins them.

There are two possibilities to consider separately, depending on whether $\psi_e(0) = 0$ or $\neq 0$. By continuity, $\psi_e(0)$ is the same for all edges e.

Beginning with the possibility that the $\psi(0) = 0$ at the central vertex, thinking of this as a fuction on a given edge e, the eigenvalues and eigenfunctions are the same as for the problem of an interval with Dirichlet conditions at one end and Neumann at the other, namely,

$$\lambda = \left(\frac{2\ell-1}{2L_e}\pi\right)^2, \ell = 1, 2, \dots$$

with an alternative way to write the eigenfunctions being

$$\psi_\ell(x_e) = A_e \sin\left(\frac{2\ell-1}{2L_e}\pi x_e\right),$$

thanks to an elementary property of sines and cosines. The Kirchhoff condition restricts the values of A_e by imposing

$$\sum_e \frac{A_e}{L_e} = 0$$

(a common factor has been dropped).

Let's think now about how many independent eigenvectors are associated with a given eigenvalue of this type. First assume that all $L_e = 1$; the general case is left as an exercise. In this case we can exploit the symmetry of the problem, by which if we permute the rôles of the edges, an eigenfunction with eigenvalue λ again becomes an eigenfunction with eigenvalue λ. By linearity, the difference of the original eigenfunction and the one with permuted edges, say e_1 and e_2, is likewise an eigenfunction, but this new eigenfunction:

- vanishes on e_3; and
- is antisymmetric along e_1 and e_2 when considered as a single interval centered at the central vertex.

We could similarly antisymmetrize in e_1 and e_3 or in e_2 and e_3, but any two of the resulting eigenfunctions can be combined to produce the third. Our conclusion is that the eigenvalues $\left(\frac{2\ell-1}{2L_e}\pi\right)^2$ have multiplicity 2.

It remains to consider the case where $\psi_e(0) \neq 0$. A simplifying trick here is to note that if the Kirchhoff condition applies to ψ, which is continuous, then it also applies to $\log\psi$, which is a way of saying that

$$\sum_e \frac{\psi_e'(0^+)}{\psi_e(0^+)} = 0.$$

This implies an equation for k,

$$\sum_e k\tan(kL_e) = 0,$$

in which the normalization factors in the eigenfunctions have disappeared and need not be thought about.

One solution is immediate, where $k = 0$ and ψ is a constant on G. For $k \neq 0$, we consider the case where all $L_e = 1$, finding that the other eigenvalues solve $\tan(k) = 0$ and are consequently of the form $\ell^2\pi^2$. These eigenvalues are simple (having a one-dimensional eigenspace), because the solution of the eigenvalue

equation is uniquely determined on each edge by its value at 0 and the fact that its derivative at 0 vanishes.

(3) **Exercise**. Consider a metric star graph with n edges of possibly different lengths L_k. Set $V = 0$. Determine the eigenvalues and their multiplicities, to the extent possible.

(4) **Exercise**. Consider the complete graph K_4 with equal edges of length 1. Set $V = 0$. Determine the eigenvalues and their multiplicities.

Examples that can be worked out by hand tend to be very symmetric and connected in a simple way. For arbitrary graphs, Sturm-Liouville theory and efficient computational methods are available to allow us to understand the solution set of a Schrödinger equation on each edge, considered by itself, but they need to be connected up according to some possibly large adjacency matrix, and it is not immediately clear how to combine the Sturm-Liouville analysis with the graph structure. To accomplish this, we borrow an idea from scattering theory, and construct a "secular determinant," as follows.

Let us consider one vertex v at a time, and orient edges outward from v, so that on each edge v lies at coordinate $x_e = 0$. We can write the conditions of continuity and the Kirchhoff condition at v in the following way. Let $\mathbf{f}$ be the vector of values of a function at 0 along edge $\mathbf{e} = 1, 2, \ldots d_v$, and let $\mathbf{f}'$ be the analogous vector of derivatives.

We can capture the continuity and Kirchhoff conditions as

$$A\mathbf{f} + B\mathbf{f}' = 0,$$

where

$$A = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ 0 & 0 & 1 & -1 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ 0 & 0 & 0 & \cdots 0 & \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}.$$

We shall work out the method under the assumption that $V = 0$, so that on each edge there is a basis of "scattering states" on any edge of the form $\exp(\pm ikx_e)$, expressing the eigenvalue parameter as $\lambda = k^2$. (In the case where $V \neq 0$ and, say, $V \geq 0$, we can make analogous arguments based on a two-dimensional basis of the solution space for the equation

$$-\psi''(x_e) + V(x_e)\psi(x_e) = k^2\psi(x_e)$$

and the corresponding *transfer matrices* $T_{\mathbf{e}}$ that connect the value and derivative of a solution at one end of a directed edge $\mathbf{e}$ with the value and derivative at its other end.)

We introduce a *scattering matrix* σ defined at a given vertex v by singling out one edge e and seeking a solution ψ of the form

$$\exp(-ikx_e) + \sigma_{ee}\exp(ikx_e)$$

on the edge e and

$$\sigma_{ee'}\exp(ikx_{e'})$$

on edges $e' \neq e$.

A calculation (see [4, 6]) shows that $A\mathbf{f} + B\mathbf{f}' = 0$ implies that, as a matrix

$$\sigma(k) = -(A + ikB)^{-1}(A - ikB). \tag{23}$$

In fact, given A and B as above, we can just choose (23) as the definition of σ, and investigate its special algebraic properties. Noticing first that $AB^* = 0$, some linear-algebra calculations show that for real $k \neq 0$,

$$(A \pm ikB)(A^* \mp ikB^*) = AA^* + k^2 BB^*.$$

This formula implies that σ is unitary (for each k):

$$\begin{aligned}
\sigma(k) &= -(A + ikB)^{-1}(A - ikB)(A^* + ikB^*)(A^* + ikB^*)^{-1} \\
&= -(A + ikB)^{-1}(A + ikB)(A^* - ikB^*)(A^* + ikB^*)^{-1} \\
&= -(A^* + ikB^*)(A^* + ikB^*)^{-1} \\
&= (\sigma(k)^*)^{-1}
\end{aligned}$$

We now construct a larger block-diagonal matrix with n blocks corresponding to the vertices v numbered in some convenient way. In the $j-th$ block we place the $d_{v_j} \times d_{v_j}$ vertex scattering matrix for v_j, which we henceforth denote σ_j:

$$\underline{\sigma}(k) := \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \vdots & \\ & & & \sigma_n \end{pmatrix}$$

The full $2m \times 2m$ *edge scattering matrix* $\underline{\sigma}(k)$ is a unitary operator on the directed edge space, and depends on k, in a way that can be made explicit with (23).

Next we write the transfer matrix in which we solve the eigenvalue equation on directed edges $\mathbf{e}$ in such a way as to connect the initial conditions at

the beginning $s\mathbf{e}$ in the basis $\exp(\pm ikx_e)$ to the values at the far end $t\mathbf{e}$ in the basis $\exp(\pm ikx_{-\mathbf{e}})$. taking care to reverse orientation, because the outward direction in which derivatives are calculated at one end of an edge is opposite to the outward direction at the other end. The entries connecting $\mathbf{e}$ and $-\mathbf{e}$ look like:

$$\begin{pmatrix} \cdots & 0 & e^{ikL_e} & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & e^{-ikL_e} & 0 & \cdots \end{pmatrix},$$

and the same thing happens at other such pairs. In this way we construct another $2m \times 2m$ unitary operator $\exp(ik\mathbf{L})$, called the *bond scattering matrix*, where the set of lengths has been organized into a vector $\mathbf{L}$.

There is a consistent solution on the entire graph where solutions connect continuously and with Kirchhoff conditions at each vertex if and only if there is a nonzero vector γ in the directed edge space such that:

$$\underline{\sigma}(k)\exp(ikL)\gamma = \gamma.$$

Linear algebra teaches us that there is a nontrivial solution of an equation of this form if and only if the *secular equation*

$$\det(I - \underline{\sigma}(k)\exp(ikL)) = 0 \tag{24}$$

has a solution. The eigenvalue problem for of H has thus been reduced to finding the roots of Eq. (24).

Verification Exercise. Write the secular equation explicitly for the examples studied above, and other small specific quantum graphs of your choosing.

6. Variations on a quantum graph

We turn our attention here to the effect on the spectrum of H when certain changes are made to a quantum graph, using, for the most part, variational methods. We begin with boundary conditions.

Suppose someone took scissors and cut a quantum graph somewhere. As we have seen, if we define a quantum Hamiltonian as the Friedrichs extension of the weak form, the newly created ends will bear Neumann conditions. One might at first think that the boundary condition poses an extra restriction on the infimum used in defining the eigenvalues, but the opposite is the case: Call the original metric graph G and the one where an edge has been cut $\tilde{G}$. Every function in the Sobolev space $H^1(G)$ is also a function in $H^1(\tilde{G})$, but the latter space also contains functions the value of which is different at the end points that are no longer joined. An

infimum of any expression over $H^1(\tilde{G})$ can only be equal to or less than the infimum of the same expression over the smaller set $H^1(G)$. Denoting the quantum graph Hamiltonian after the cut $\tilde{H}$, since the weak forms of H ands $\tilde{H}$ are identical, but $H^1(G) \subset H^1(\tilde{G})$, it follows from the min-max principle that $\lambda_j(\tilde{H}) \leq \lambda_j(H)$. I.e., imposing an extra Neumann condition can never increase any eigenvalue of the Hamiltonian. (The argument is perhaps easier to follow using the form of min-max given in Theorem 3 than in Theorem 2.) The same argument shows that if we change the conditions at a vertex from Kirchhoff to Neumann, as if we cut the edges loose there, eigenvalues can only decrease or remain unchanged.

The other standard type of boundary condition for ordinary differential equations is Dirichlet, which in the homogeneous form means classically that a function is forced to be zero on some boundary point. In the weak definition of a differential operator, Dirichlet boundary conditions are what results when a Sobolev space is defined as the completion of smooth functions that vanish in a neighborhood of the set on which Dirichlet conditions are imposed. Without needing to go into details of this construction, we can understand that, just as a matter of set theory, the new Sobolev space is a subset of $H^1(G)$. Any infimum can only be pushed up by searching over a smaller set, so it follows that imposing an extra Dirichlet condition can never *decrease* any eigenvalue of the Hamiltonian.

An interesting consequence of the technique of *Dirichlet-Neumann bracketing*, which estimates eigenvalues above and below imposing extra boundary conditions of the two types, has to do with the *Weyl law* for eigenvalues. Again we set $V = 0$, although it is not hard to determine how Weyl's formula is altered to incorporate a potential energy.

The eigenvalue problem for an interval of length L with Dirichlet conditions at the ends is elementary, and the eigenvalues are found to be $\lambda_j = (j\pi/L)^2$, $j = 1, 2, \ldots$, tending to $+\infty$. The eigenvalues for the same interval with Neumann boundary conditions are likewise $\lambda_j = (j\pi/L)^2$, except that now $j = 0, 1, 2, \ldots$, tending to $+\infty$. If you prefer to ask how many eigenvalues are $\leq k^2$, the answer is $N(k) = (L/\pi)k + 0(1)$, with either Dirichlet or Neumann conditions. Critically, this estimate of the eigenvalue-counting function $N(k)$ will be true even if we have a union of independent intervals, where L denotes the total length, because each interval contributes the same estimate in proportion to its length. Now, a quantum-graph Hamiltonian with $V = 0$, i.e., a quantum-graph Laplacian, can be converted into effectively disjoint intervals by changing the vertex

conditions to either Dirichlet (pushing eigenvalues up) or Neumann (pushing them down). Since both the lower and upper bound have the same asymptotic form, so does $N(k)$ for the graph. This establishes the Weyl law for finite graphs:

Theorem 8. *Let H be a quantum-graph Laplacian on a metric graph G with total length L, and denote its eigenvalue-counting function $N(k) :=$ the number of eigenvalues $\leq k^2$. Then*

$$N(k) = \frac{Lk}{\pi} + O(1),$$

and therefore

$$\lambda_j \sim \left(\frac{\pi j}{L}\right)^2$$

as $j \to \infty$.

Exercise. Consider two metric graphs that consist of the same edges bearing the same potential energy functions $V(x_e)$, but connected in different ways. Show that the eigenvalues λ_j of their Hamiltonians have the same asymptotic behavior as $j \to \infty$. Determine to the leading-order how V appears in this asymptotic behavior.

Another alteration of a quantum graph we can consider is the coalescence of two vertices into one, to which all edges that connected to either of the original vertices now connect. What effect does this have on the eigenvalues? The answer to this is another interlacing theorem:

Theorem 9. *Let two graphs have the same edges and the same potential-energy functions V, but suppose that a pair of vertices v_1 and v_2 of G_a have been identified in G_b, with Kirchhoff conditions applying now to the union of the sets of edges connecting in G_a to v_1 and to v_2. Let the eigenvalues of the corresponding Hamiltonians be denoted λ_j^a and λ_j^b, $j = 1, 2, \ldots$. Then for all j,*

$$\lambda_j^a \leq \lambda_j^b \leq \lambda_{j+1}^a. \tag{25}$$

Proof. The first inequality follows from a similar argument as the one establishing what happens when a Dirichlet or Neumann condition is imposed in a graph. The continuity required in the Sobolev space for G_b requires functions from the full set of edges to attain the same value at the points where they attach to the conjoined vertex, whereas in the Sobolev space for G_a less continuity is required. (There is continuity at v_1 and v_2, but no requirement that the values at the two vertices be the same.) The weak

forms for the two Hamiltonians are identical, but the set over which we seek the infimum for λ_j^b is a subset of that for λ_j^a, implying that $\lambda_j^b \geq \lambda_j^a$.

For the other inequality, we shall cook up j orthonormal test functions for H_b, each of which satisfies

$$\frac{\langle H\varphi, \varphi\rangle}{\|\varphi\|^2} \leq \lambda_{j+1}^a.$$

We begin with the set $\{\phi_1 \cdots \phi_{k+1}\}$ of orthonormalized eigenfunctions for H_a corresponding to the eigenvalues $\{\lambda_1^a \cdots \lambda_{k+1^a}\}$. The problem with these is that they do not necessarily have the same values at v_1 as at v_2. If by accident some of the first $j+1$ eigenfunctions for H_a satisfy $\phi_i(v_1) = \phi_i(v_2)$, say $p \leq j$ of them, we relabel them as φ_i, $i = 1, \ldots, p$. The remaining $j+1-p$ differ at the two vertices, so we reorder them as ϕ_{ℓ_i}, $i = p+1, \ldots j+1$, and then construct combinations

$$\tilde{\phi}_{p+1} := \phi_{\ell_{p+1}} - \alpha_{p+1}\phi_{\ell_{j+1}},$$

with a constant chosen so that $\tilde{\phi}_{p+1}(v_1) = \tilde{\phi}_{p+1}(v_2)$. We next take a function of the form $\phi_{\ell_{p+2}} - \alpha_{p+2}\ \phi_{\ell_{j+1}}$ where α_{p+2} is chosen so that the values at v_1 and v_2 are the same, and then define $\tilde{\phi}_{p+2}$ as the projection of that function orthogonal to $\tilde{\phi}_{p+1}$ This is guaranteed not to be identically 0 because of the independence of the functions $\phi_{\ell_{p+1}}, \phi_{\ell_{p+2}}$, and $\phi_{\ell_{j+1}}$, and it still satisfies $\tilde{\phi}_{p+2}(v_1) = \tilde{\phi}_{p+2}(v_2)$. We continue in this manner, first subtracting a multiple of $\phi_{\ell_{j+1}}$ from $\phi_{\ell_{p+s}}$ to make the values at v_1 and v_2 equal, and then projecting onto the orthogonal complement of the span of $\phi_{\ell_{p+1}}, \ldots, \phi_{\ell_{p+s-1}}$ to define a nonzero $\tilde{\phi}_{p+s}$, stopping when $p+s = j$. For $i = p+1$ to j, we let

$$\varphi_i := \frac{\tilde{\phi}_i}{\|\tilde{\phi}_i\|}.$$

By a direct calculation, the j orthonormal functions φ_i are in the quadratic-form domain of H_b and each satisfy $\langle H_b\varphi_i, \varphi_i\rangle \leq \lambda_{j+1}^a$, so the min-max principle implies that $\lambda_j^b \leq \lambda_{j+1}^a$. □

The alert reader will have noticed the similarity between the argument to establish the second inequality and the Courant-Weyl formula 14.

This has been but a sampling of what is known about the eigenvalues of quantum graphs, in the case where they are discrete, and we have not even touched on questions of scattering theory, resonances, etc., which are

among the most important topics when the graph is infinite and has essential spectrum. The motivated reader is encouraged to go deeper into the subject beginning with the excellent monographs [4, 6].

Here are a few open challenges for the future:

(1) Are there spectral conditions on a quantum-graph Hamiltonian that determine the graph and the potential energy uniquely?
(2) Do the effects of the graph structure and the potential show up differently in the spectrum, or can the graph structure be considered an "effective potential"?
(3) What "universal" constraints characterize the possible spectra, independently of the potential? Independently of the connectedness? What does the set of possible spectra of, say a graph of given total edge length, look like?
(4) Are there systematic ways of contructing cospectral sets of quantum graphs?
(5) What metric graph maximizes or minimizes λ_j for the Laplacian, given, for example, a fixed total edge length and number of edges? How about other spectral quantities such as the trace of the heat kernel? (For analogous questions for Laplacians on domains and manifolds, whch could offer guidance, see [34].)

7. Eigenfunctions of quantum graphs

In this final section we'll briefly consider the other side of spectral theory, namely the eigenfunctions, rather than the eigenvalues.

Harkening back to the spectral theory of Laplacian and Schrödinger operators, precise knowledge of even one eigenfunction ψ allows one to determine the domain or the potential energy, up to minor details, simply by plugging into the eigenvalue equation and dividing by ψ, since elliptic equations have unique continuation theorems (Ee.g., [20]), which ordinarily prevent ψ from vanishing on any open set. In other words, knowing one eigenfunction means knowing everything there is to know about the operator.

The situation is not as straightforward on graphs, whether combinatorial or metric, since it is possible for eigenfunctions to vanish on significant parts of the graph. We have seen this in the discrete case with the eigenfunctions $h_{u\vec{v}}$ of the complete graph, which differ from 0 only on two vertices. It is also quite common on quantum graphs for an eigenfunction to vanish on entire edges.

Here is a simple way to construct examples to illustrate this phenomenon on a quantum graph. Consider any quantum-graph Hamiltonian H on a

metric graph G, where the eigenfunction changes sign, vanishing at some point x_0 (On a connected graph, there can be only one independent eigenfunction that fails to vanish somewhere, because the set of eigenfunctions can be orthogonalized.) Now create a second copy of H, G, on which we shall designate the equivalent point $\hat{x}_0$. Now connect the two copies of G with *any graph whatsoever* that meets the original graphs only at x_0 and $\hat{x}_0$. Put *any potential whatsoever* on the connecting graph. The function which equals the original eigenfunction on the the two copies of G and is identically zero on the connecting graph is an eigenfunction of the quantum-graph Hamiltonian that has thus been created.

A major barrier to the use of eigenfunctions to determine a quantum graph is that calculating an eigenfunction precisely enough to differentiate is not easy in practice, and it can be computationally burdensome. Moreover, a complex graph may not be known in detail. What is really needed, both for applications and for proving general theorems, is efficient ways of identifying features of eigenvectors or eigenfunctions, especially

- Localization (especially on infinite graphs), i.e., ways to know when the eigenfunctions are confined to compact regions, or at least in some L^p spaces, as opposed to being "extended states."
- *Nodal domains*, i.e., subdomains where the eigenvector has one sign or the other, as well as zero sets as mentioned above.
- Local regions where the eigenfunctions in a given energy range are small.

Ideally, these features should be connected with the graph structure and the potential energy.

Eigenvectors on combinatorial graphs are the subject of a short monograph [8], but many questions remain open. Among the interesting more recent advances in understanding these eigenvectors are the investigations by Berkolaiko [5] and Colin de Verdi‘ere [17] of the number of nodal domains by introducing magnetic perturbations. (This method has also been used to count nodal domains for quantum graphs in [7].)

The subject of the eigenfunctions of quantum-graph Hamiltonians is even less developed. One topic of current research is the problem of trying to locate regions where eigenfunctions are small in magnitude and regions where they may be large. One way in which this subject has been approached in other contexts than quantum graphs is through the identification of a *landsape function* $\Upsilon(x, \lambda) > 0$ [29, 42], for which it can be shown that any

eigenfunction $\psi(x)$ with eigenvalue λ must satisfy

$$|\psi(x)| \leq \Upsilon(x, \lambda).$$

Obviously, the smaller the landscape function is, the better, and it only becomes interesting if it is really is like a landscape, with mountains and valleys that truly show where the eigenfunctions are concentrated and where they are excluded.

Various methods have been advanced to produce landscape functions, for example based on probabilistic analysis or on the maximum principle [42], which, as we know from §1 has deep connections to Laplacians. Here we make some remarks on how the use of the maximum principle can be adapted to the setting of quantum graphs, following [32].

Lemma 1. *Let H be a quantum-graph Hamiltonian with $V(x) \geq 0$ on an open subset $\mathcal{S}$ of G. Suppose that $w \in C^2$ and that $Hw := -w'' + V(x)w$ on edges, with Kirchhoff conditions at the vertices. If $Hw \leq 0$ on the edges contained in $\mathcal{S}$, then $w_+ := max(w, 0)$ does not have a strict local maximum on $\mathcal{S}$.*

Proof. We follow a standard proof by contradiction of the maximum principle for elliptic partial differential equations, except that we need to take care about the vertices.

For this purpose we may assume that $w > 0$ at the putative maximum, as the value 0 cannot logically be a strict local maximum value of w_+. We next argue that it suffices to prove the maximum principle under the assumption that $Hw \leq -\epsilon^2$ on $\mathcal{S}$ for some $\epsilon \neq 0$, since if w has a strict local maximum on $\mathcal{S}$, then so does $w_\delta(x) := \exp(\delta x)w(x)$ for sufficiently small $|\delta(x)|$, at a point $x_1 \in \mathcal{S}$. But $Hw_\delta(x) = \exp(\delta x)\left(-\delta^2 w - \delta w' + Hw\right)$, and therefore for δ of sufficiently small magnitude and with the same sign as $w'(x_1)$ (if nonzero), this will be strictly negative in a neighborhood of x_1.

Thus we posit without loss of generality that $Hw \leq -\epsilon^2$ for some $\epsilon > 0$. If we suppose that w is maximized at some x_0 interior to an edge, then $w'(x_0) = 0$ and $w''(x_0) \leq 0$, but this contradicts the assumption that $Hw \leq -\epsilon^2$. If on the other hand the maximixing x_0 is a vertex, then for each edge e emanating from x_0, $w'_e(x_0^+) \leq 0$. Because of the Kirchhoff conditions, if for any edge, $w'_e(x_0^+) < 0$, there must be at least one other edge e' on which $w'_{e'}(x_0^+) > 0$, which would contradict maximality. Therefore $w'_e(x_0^+) = 0$ for all e, and a necessary condition for maximality is then that $w''_e(x_0^+) \leq 0$. This, however contradicts $Hw \leq -\epsilon^2$. □

A landscape function proposed in [29] for the analogous problem on a domain in $\mathbb{R}^d$ is a multiple of the solution to of $(-\Delta+V(x))U = 1$, sometimes known as a *torsion function*. In fact it would suffice to have a solution of $(-\Delta + V(x))U \geq 1$ on some open set $\mathcal{S}$ for this purpose, which adds some flexibility. This also works for the case of quantum graphs [32], by the following observation.

Let $w(x) := \pm\psi(x) - \lambda CU(x)$. Since

$$Hw = \lambda(\pm\psi - C),$$

we can ensure that $Hw \leq 0$ if C is sufficiently large. (C could be $\|\psi\|_{L^\infty(\mathcal{S})}$ or one of the general upper bounds on this quantity available in the literature.) By the maximum principle, w_+ cannot have an interior maximum, and therefore

$$|\psi(x)| \leq \Upsilon(x) + \sup_{\partial\mathcal{S}}(|\psi(x)| - \Upsilon(x))_+$$

throughout $\mathcal{S}$, where $\Upsilon = \lambda CU(x)$.

Let em close with a few final open challenges related to the eigenfunctions.

(1) What sharp, explicit landscape functions can be created for quantum graphs, and how do they connect the regions where eigenfunctions concentrate both to the potential energy and to features of the graph? For instance, Laplacian eigenvectors on combinatorial graphs are used to identify clusters [2, 28]. Do eigenfunctions of quantum graphs pick out analogous features?

(2) How is the quantum tunneling effect affected by the topology of a quantum graph? It was shown in [31], using the Agmon method, that exponential tunneling bounds for localizing low-energy eigenfunctions on the line apply unchanged to quantum-graph Hamiltonians, but that, often, a graph structure can enhance the localization. Can these bounds be made more explicit, and can they be adapted to the high-energy case? Is it possible to identify particular topological features of a quantum graph that strongly enhance the tunneling effect of the potential?

(3) How can tunneling estimates and landscape functions be adapted to control the eigenfunctions of combinatorial graphs? (See [21, 16] for some work related to this topic.)

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