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The Graph Laplacian

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Definition of the Graph Laplacian

Let (V, E) be a directed graph. Assume that there are at most M edges joining any vertex. For $p, q \in V$, let pq denote a directed edge with initial vertex p and final vertex q. Define the operator

$$d : \ell^2(V) \to \ell^2(E)$$

by

$$(d\varphi)(pq) = \varphi(q) - \varphi(p)$$

Then d is a bounded operator with bound at most $2\sqrt{M}$. To compute the adjoint d^* we use the fact that every edge starts at exactly one vertex, and also ends at exactly one vertex. Thus we can write a sum over all edges in two ways as

$$\sum_{pq \in E} = \sum_{r \in V} \sum_{\substack{pq \in E \\ q=r}} = \sum_{r \in V} \sum_{\substack{pq \in E \\ p=r}}$$

Thus

$$
\begin{aligned}
\langle \psi, d\varphi \rangle &= \sum_{pq \in E} \overline{\psi}(pq) d\varphi(pq) \\
&= \sum_{pq \in E} \overline{\psi}(pq)\varphi(q) - \sum_{pq \in E} \overline{\psi}(pq)\varphi(p) \\
&= \sum_{r \in V} \sum_{\substack{pq \in E \\ q=r}} \overline{\psi}(pq)\varphi(r) - \sum_{r \in V} \sum_{\substack{pq \in E \\ p=r}} \overline{\psi}(pq)\varphi(r) \\
&= \sum_{r \in V} \left(\sum_{\substack{pq \in E \\ q=r}} \overline{\psi}(pq) - \sum_{\substack{pq \in E \\ p=r}} \overline{\psi}(pq) \right) \varphi(r)
\end{aligned}
$$

This implies that d^* is given by

$$(d^*\psi)(r) = \sum_{\substack{pq \in E \\ q=r}} \psi(pq) - \sum_{\substack{pq \in E \\ p=r}} \psi(pq)$$

A conductivity γ is a positive function on E. We also denote by γ the corresponding multiplication operator on $\ell^2(E)$ (i.e., the diagonal matrix with the entries of γ on the diagonal.) The Laplacian is defined by

$$\Delta_\gamma = d^*\gamma d.$$

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If γ is a bounded function then the Laplacian is a non-negative bounded self-adjoint operator. Notice that

$$\begin{aligned}(\Delta_\gamma\varphi)(r) &= \sum_{\substack{pq\in E\\q=r}} \gamma(pq)(d\varphi)(pq) - \sum_{\substack{pq\in E\\p=r}} \gamma(pq)(d\varphi)(pq)\\ &= \sum_{\substack{pq\in E\\q=r}} \gamma(pq)(\varphi(q)-\varphi(p)) - \sum_{\substack{pq\in E\\p=r}} \gamma(pq)(\varphi(p)-\varphi(q))\\ &= \sum_{q\in N(r)} \gamma(rq)(\varphi(r)-\varphi(q))\end{aligned}$$

Here $N(r)$ denotes the set of nearest neighbours of r in V. Notice that the definition of the Laplacian is insensitive to the directions of the arrows on the edges.

Graphs with boundary and the Dirichlet problem

A graph with boundary is a graph with a distinguished subset V_b of vertices called boundary vertices. The set of interior vertices V_i is the complement $V_i = V \setminus V_b$. We will assume that the boundary is non-empty and that the graph is connected.

We may decompose $\ell^2(V) = \ell^2(V_i) \oplus \ell^2(V_b)$. Let P and Q be the corresponding orthogonal projections. For $u \in \ell^2(V)$, the boundary value of u is Qu, while the discrete analogue of the normal derivative is $Q\Delta u$.

Given $f \in \ell^2(V_b)$ and $\lambda \in \mathbb{C}$ we will consider the following Dirichlet problem: find $u \in \ell^2(V)$ solving

$$P(\Delta - \lambda)u = 0$$
$$Qu = f \tag{1.1}$$

To solve the Dirichlet problem introduce the Dirichlet Laplacian

$$\Delta_D = P\Delta P$$

The Dirichlet Laplacian is clearly self-adjoint and non-negative, since Δ is. In fact, Δ_D is strictly positive, since $\Delta_D u = 0$ implies $dPu = 0$ so that Pu is constant. But Pu is zero on the boundary. This implies u is identically zero. Let $\sigma(\Delta_D)$ denote the spectrum of Δ_D.

The unique solvability of the Dirichlet problem depends on whether λ is in the spectrum of Δ_D. Clearly, if λ is an eigenvalue, we may add the corresponding eigenfunction to any solution, so we lose uniqueness. On the other hand, if $\lambda \notin \sigma(\Delta_D)$ then any solution u satifies

$$P(\Delta - \lambda)Pu = -P\Delta Qu$$

because $P + Q = 1$ and $PQ = 0$. The assumption on λ means we may invert the operator on the left, so that

$$Pu = -P(\Delta_D - \lambda)^{-1}P\Delta Qu$$

Thus

$$u = Qu - P(\Delta_D - \lambda)^{-1}P\Delta Qu$$
$$= Qf - P(\Delta_D - \lambda)^{-1}P\Delta Qf$$

(1.2)

By reversing these steps we can obtain the following proposition.

Proposition 1.1 *The Dirichlet problem (1.1) has a unique solution if and only if $\lambda \notin \sigma(\Delta_D)$*

Notice that by strict positivity, 0 is never in $\sigma(\Delta_D)$. This implies that the Dirichlet problem always has a solution for $\lambda = 0$.

The Dirichlet to Neumann map

The Dirichlet to Neumann map $\Lambda(\lambda) : \ell^2(V_b) \to \ell^2(V_b)$ is define for every $\lambda \notin \sigma(\Delta_D)$ as

$$\Lambda(\lambda)f = Q\Delta u$$

where u solves the Dirichlet problem (1.1).

If $\lambda \in \mathbb{R} \backslash \sigma(\Delta_D)$ then $\Lambda(\lambda)$ is self-adjoint. This follows from the discrete analogue of Green's formula. To derive this, start with

$$\langle u, \Delta v \rangle - \langle \Delta u, v \rangle = 0$$

Now introduce $I = P + Q$ to obtain

$$\langle u, P\Delta v \rangle - \langle P\Delta u, v \rangle = -\langle u, Q\Delta v \rangle + \langle Q\Delta u, v \rangle.$$

Adding and subtracting $\langle u, P\lambda v \rangle = \langle P\lambda u, v \rangle$ (here we use that λ is real) to the left side yields

$$\langle u, P(\Delta - \lambda)v \rangle - \langle P(\Delta - \lambda)u, v \rangle = -\langle u, Q\Delta v \rangle + \langle Q\Delta u, v \rangle.$$

which is the discrete version of Green's formula.

Now, if u solves the Dirichlet problem (1.1) and v solves the same problem with f replaced by g, then $P(\Delta - \lambda)u = P(\Delta - \lambda)v = 0$, $Q\Delta u = \Lambda(\lambda)f$ and $Q\Delta u = \Lambda(\lambda)g$. Therefore

$$\langle f, \Lambda(\lambda)g \rangle = \langle \Lambda(\lambda)f, g \rangle$$

which proves the symmetry of $\Lambda(\lambda)$.

Another useful formula that follows from $P(\Delta - \lambda)u = 0$ is

$$\|\gamma du\|^2 = \langle u, (\Delta - \lambda)u \rangle + \lambda \langle u, u \rangle = \langle u, Q\Delta u \rangle + \lambda \langle u, Pu \rangle$$

Thus implies

$$\langle f, \Lambda(\lambda)f \rangle = \|\gamma du\|^2 - \lambda \|Pu\|^2$$

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where u solves (1.1). This formula is used the the PDE context to define $\Lambda(\lambda)$ as a quadratic form. It shows that $\Lambda(0) \geq 0$.

In our discrete situation, the above calculations are somewhat superfluous, since we can obtain a formula for $\Lambda(\lambda)$. If follows from (1.2) that

$$\Lambda(\lambda) = Q\Delta Q - Q\Delta P(\Delta_D - \lambda)^{-1}P\Delta Q \tag{1.3}$$

This formula shows that for a finite graph $\Lambda(\lambda)$ is a rational function whose poles may only occur at the eigenvalues of Δ_D.

Inverse problems for the Dirichlet to Neumann map

This was the subject of an undergraduate research project by **Kyle Eliot**.

Let us fix a graph with boundary. There are several inverse problems associated with the Dirichlet to Neumann map:

(a) Does knowledge of $\Lambda(0)$ determine the conductivity γ?

(b) Does knowledge of $\Lambda(\lambda)$ for all λ determine the conductivity γ?

One may also consider the more difficult problem where only the boundary of the graph is fixed, and we seek to determine the interior of the graph as well.

If the graph with conductivities is modeling a resistor network, where V_b are the nodes accessible to measurement, then (a) corresponds to the experiment of applying a steady voltage distribution f and measuring the current after a steady state has been reached. This current distribution is $\Lambda(0)f$ so making all possible such measurement is equivalent to knowing $\Lambda(0)$. Of course it is enough to do this for f in some basis of $\ell^2(V_b)$.

We may also consider the situation where we may apply time varying voltages and measure the resulting time varying currents. Assume that the voltage $u(t)$ is modeled by the discrete wave equation

$$P(\Delta + \frac{\partial^2}{\partial t^2})u(t) = 0$$
$$Qu(t) = f(t)$$

where $f(t)$ is the applied voltage and $Q\Delta u(t)$ is measured current. Taking the Fourier transform in t converts this problem to

$$P(\Delta - k^2)\hat{u}(k) = 0$$
$$Q\hat{u}(k) = \hat{f}(k)$$

where we are given $\hat{f}(k)$ and measure $Q\Delta\hat{u}(k) = \Lambda(k^2)\hat{f}(k)$. Thus this inverse problem corresponds to (b).

It is clear that unless there is some restriction on the graph, the answer to (a) is no. For example, if the boundary has a single node, we will not be able to recover a large number of

conductivities. Thus the problem becomes to characterize for which graphs the answer is yes. The answer is not simple, and has been studied, for example, by James Morrow, his students and collaborators. (`http://www.math.washington.edu/~morrow/reu02/reu.html` contains a collection of papers of various discrete inverse problems).

The problem (b) is easier, since we are given more information. Suppose we know $\Lambda(\lambda)$ for all λ. Starting with the formula (1.3) we may make a Neumann expansion.
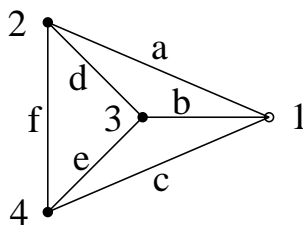
$$\begin{aligned}
\Lambda(\lambda) &= Q\Delta Q - Q\Delta P(\Delta_D - \lambda)^{-1}P\Delta Q \\
&= Q\Delta Q + \lambda^{-1}Q\Delta P(1 - \Delta_D/\lambda)^{-1}P\Delta Q \\
&= Q\Delta Q + \lambda^{-1}Q\Delta P\sum_{k=0}^{\infty}\Delta_D^k\lambda^{-k}P\Delta Q \\
&= Q\Delta Q + \sum_{k=0}^{\infty}\lambda^{-k-1}Q\Delta P(P\Delta P)^k P\Delta Q
\end{aligned}$$

This expansion converges for $|\lambda| > \|\Delta_D\|$. Since we can recover the analytic function $\Lambda(\lambda)$ from the coefficients in this expansions, we find the knowing $\Lambda(\lambda)$ for all λ is equivalent to knowing $Q\Delta Q$ and $Q\Delta P(P\Delta P)^k P\Delta Q$ for $k = 0, 1, 2, \ldots$.

Notice that we can immediately read off the conductivities for edges that join two boundary vertices. These are simply the off-diagonal elements of $Q\Delta Q$. On the other hand, they don't appear in the other given information $Q\Delta P(P\Delta P)^k P\Delta Q$ for $k = 0, 1, 2, \ldots$. Thus, we may as well assume that all the intra-boundary conductivities are zero. If we can do this case, we can also solve the general case. Notice that setting a conductivity to zero is same as simply eliminating that edge in the graph.

This observation also motivates our approach to studying non-uniqueness. We will begin with a graph that contains all possible edges, except the ones between two boundary vertices. It turns out that the local deformations of γ preserving the function $\Lambda(\lambda)$ are given by the orthogonal group acting on γ. This action does not neccesarily preserve the positivity of γ, though. Deleting an edge puts a constraint on this action. So we expect that if we delete enough edges we should achieve rigidity.

Let's study the simplest case in detail. Consider the complete graph with four vertices.

With a suitable labelling of the edges, $\gamma = \operatorname{diag}[a, b, c, d, e, f]$ and

$$\Delta = \begin{bmatrix} a+b+c & -a & -b & -c \\ -a & a+d+f & -d & -f \\ -b & -d & b+d+e & -e \\ -c & -f & -e & c+e+f \end{bmatrix}$$

The Dirichlet Laplacian is bottom right 3×3 block:

$$\Delta_D = \operatorname{diag}[a, b, c] + \begin{bmatrix} d+f & -d & -f \\ -d & d+e & -e \\ -f & -e & e+f \end{bmatrix}$$

$$= D + \Delta_0$$

where Δ_0 is the graph Laplacian for the interior of the graph. Let

$$X = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Then $\Delta_0 X = 0$ so that $Q\Delta Q$ (which, in the case of one boundary node, is a number) can be written

$$Q\Delta Q = \langle X, DX \rangle = \langle X, D + \Delta_0 X \rangle = \langle X, \Delta_D X \rangle$$

Similarly

$$Q\Delta P(P\Delta P)^k P \Delta Q = \langle X, D\Delta_D^k DX \rangle = \langle X, (D + \Delta_0)\Delta_D^k(D + \Delta_0)X \rangle = \langle X, \Delta_D^{k+2} X \rangle$$

Thus we find that knowledge of $\Lambda(\lambda)$ for all λ is the same as the knowledge of $\langle X, \Delta_D^k X \rangle$ for $k = 1, 2, 3, \ldots$.

Now it is easy to see how to make a deformation that preserves $\Lambda(\lambda)$. Let O be an orthogonal matrix fixing X. Then clearly $\langle X, \Delta_D^k X \rangle = \langle X, \tilde{\Delta}_D^k X \rangle$ where $\tilde{\Delta}_D = O^T L_D O$. The only question is whether $\tilde{\Delta}_D$ is the Dirichlet Laplacian arising from a graph with postive conductivities. This will be the case if the off-diagonal entries are all negative and row sums are all positive.

In the present example, the group of orthogonal matrices preserving X is one dimensional, i.e., a circle. We can explicitly compute the deformations starting with any $\gamma = \operatorname{diag}[a, b, c, d, e, f]$.
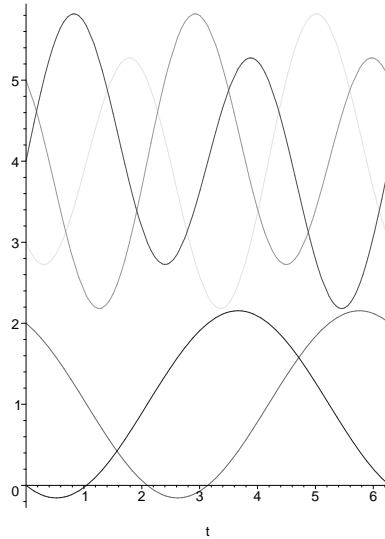
Suppose we are interested in the graph with an edge removed. We set, for example $\gamma = \operatorname{diag}[0, 1, 1, 1, 1, 2]$ corresponding to the graph
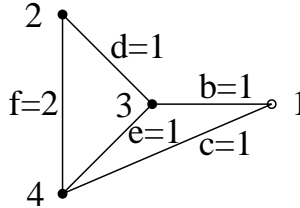
Then the deformations look like
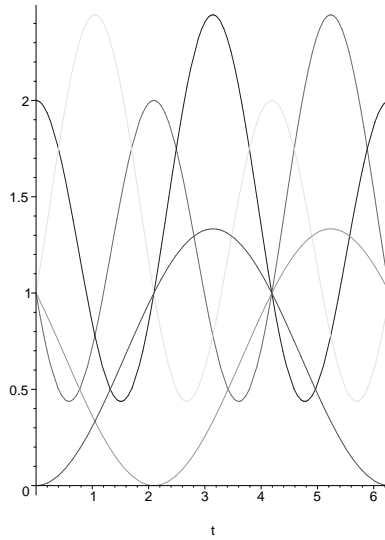
In this case we see that none of these deformations have $a = 0$ However, if we start with $\gamma = \mathrm{diag}[1, 2, 3, 4, 0, 1]$ the resulting deformations look like

In this case, there is another value of the conductivities amongst the deformations with $e = 0$ and all the rest positive. So even though we have local rigidity, there are two distinct conductivities for the graph with the edge labeled by e missing which give rise to the same $\Lambda(\lambda)$.

The general case with one boundary node.

The general case.

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Lagrangian subspaces and self-adjoint operators

We review the connection between Lagrangian subspaces and self-adjoint operators. Let X be an n dimensional vector space over $\mathbb{C}$ with inner product $\langle \cdot, \cdot \rangle$. Consider $X \oplus X$ with the inner product

$$\left\langle \begin{bmatrix} w \\ x \end{bmatrix}, \begin{bmatrix} y \\ z \end{bmatrix} \right\rangle = \langle w, y \rangle + \langle x, z \rangle$$

Let $J : X \oplus X \to X \oplus X$ be given in block form by

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

Then the standard symplectic form ω on $X \oplus X$ is given by

$$\omega \left[\begin{bmatrix} w \\ x \end{bmatrix}, \begin{bmatrix} y \\ z \end{bmatrix} \right] = \left\langle \begin{bmatrix} w \\ x \end{bmatrix}, J \begin{bmatrix} y \\ z \end{bmatrix} \right\rangle = \langle w, z \rangle - \langle x, y \rangle$$

Given a subspace $L \subseteq X \oplus X$, define the skew-complement L^ω to be

$$L^\omega = \left\{ \begin{bmatrix} w \\ x \end{bmatrix} : \left\langle \begin{bmatrix} w \\ x \end{bmatrix}, J \begin{bmatrix} y \\ z \end{bmatrix} \right\rangle = 0 \text{ for every } \begin{bmatrix} y \\ z \end{bmatrix} \in L \right\}$$

Clearly $L^\omega = JL^\perp$, where $L^\perp$ is the usual orthogonal complement.

A subspace L is called isotropic if $L \subseteq L^\omega$, co-isotropic if $L^\omega \subseteq L$ and Lagrangian if it is both isotropic and co-isotropic, so that $L = L^\omega$. An isotropic subspace L is Lagrangian if it is maximal (not contained in a larger isotropic subspace), or equivalently, if its dimension is n. Similarly, a co-isotropic subspace L is Lagrangian if it is minimal (not containing a smaller co-isotropic subspace), or equivalently, if its dimension is n.

In this complex setting, the Lagrangian subspaces can be parametrized by the unitary group $U(n)$. To do this, we first note that J has eigenvalues $\pm i$ with n dimensional eigenspaces $K_\pm$. For $z \in X \oplus X$ let $z = z_+ + z_-$ denote the orthogonal decomposition with $z_\pm \in K_\pm$. Then for each unitary map $U : K_+ \to K_-$ we associate the Lagrangian supspace

$$L_U = \{z \in X \oplus X : z_- = Uz_+\}$$

Proposition 1.2 *The correspondence $U \mapsto L_U$ gives a parametrization of all the Lagrangian subspaces.*

Proof: First we show that L_U is Lagrangian for every unitary U. Clearly L_U is n dimensional, so we need only show it is isotropic. But if $z, w \in L_U$, then

$$\omega[z, w] = \langle z, Jw \rangle = i \langle z_+, w_+ \rangle - i \langle z_-, w_- \rangle = i \langle z_+, w_+ \rangle - i \langle Uz_+, Uw_+ \rangle = 0,$$

since U is unitary.

Now suppose L is Lagrangian. Then $z \in L$ implies

$$\omega[z, z] = \langle z, Jz \rangle = i\|z_+\|^2 - i\|z_-\|^2 = 0,$$

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so $\|z_+\| = \|z_-\|$. Thus the projection $P_+ : L \to K_+$ restricted to L has no kernel. Since $\dim(L) = \dim(K_+)$ it is an isomorphism. Similarly, $P_- : L \to K_-$ is an isomorphism and so the composition of the inverse of the restriction of P_+ with P_- gives an isomorphism $U : K_+ \to K_-$ such that $z_+ + Uz_+ \in L$. This implies $\|Uz_+\| = \|z_+\|$ for every $z_+ \in K_+$ so we find that U is unitary. $\square$

Another way of describing Lagrangian subspaces is via two linear transformations $A, B : X \to X$ with AB^* self-adjoint (hermitian). Define

$$L_{A,B} = \left\{ \begin{bmatrix} w \\ x \end{bmatrix} \in X \oplus X : Aw + Bx = 0 \right\}$$

Then $L_{A,B}$ is kernel of the linear transformation $X \oplus X \to X$ given in block form by $\begin{bmatrix} A & B \end{bmatrix}$. Thus

$$L_{A,B}^\omega = JL_{A,B}^\perp = J\operatorname{Ker}\left(\begin{bmatrix} A & B \end{bmatrix}\right)^\perp = J\operatorname{Ran}\left(\begin{bmatrix} A^* \\ B^* \end{bmatrix}\right) = \left\{ \begin{bmatrix} B^*x \\ -A^*x \end{bmatrix} : x \in X \right\}$$

Since AB^* is hermitian, $AB^*x - BA^*x = 0$. This implies $L_{A,B}^\omega \subseteq L_{A,B}$ so that $L_{A,B}$ is co-isotropic. If, in addition, $\begin{bmatrix} A & B \end{bmatrix}$ has maximal rank, so that $\dim\left(\operatorname{Ker}\left(\begin{bmatrix} A & B \end{bmatrix}\right)\right) = n$ then $L_{A,B}$ is Lagrangian.

To understand the connection between these descriptions we first identify unitary maps U from $K_+ \to K_-$ with unitary matrices $\tilde{U} \in U(n)$. We have

$$K_\pm = \left\{ \begin{bmatrix} x \\ \pm ix \end{bmatrix} : x \in X \right\}$$

and unitary maps $U : K_+ \to K_-$ can be written

$$U \begin{bmatrix} x \\ ix \end{bmatrix} = \begin{bmatrix} \tilde{U}x \\ -i\tilde{U}x \end{bmatrix}$$

for some $\tilde{U} \in U(n)$. The projections $P_\pm$ onto $K_\pm$ have the form

$$P_\pm \begin{bmatrix} x \\ y \end{bmatrix} = \frac{1}{2} \begin{bmatrix} x + iy \\ \pm i(x \pm iy) \end{bmatrix}$$

Thus

$$\begin{bmatrix} x \\ y \end{bmatrix} \in L_U \iff P_- \begin{bmatrix} x \\ y \end{bmatrix} = UP_+ \begin{bmatrix} x \\ y \end{bmatrix}$$
$$\iff \begin{bmatrix} x - iy \\ -i(x - iy) \end{bmatrix} = \begin{bmatrix} \tilde{U}(x + iy) \\ -i\tilde{U}(x + iy) \end{bmatrix}$$
$$\iff (x - iy) = \tilde{U}(x + iy)$$
$$\iff (I - \tilde{U})x - i(I + \tilde{U})y = 0$$

Thus $L_U = L_{A,B}$ with $A = (I - \tilde{U})$ and $B = -i(I + \tilde{U})$.

By considering the special case is where A is self-adjoint and $B = I$, we see that the graph of any self-adjoint operator is a Lagrangian subspace. Conversely, if B is invertible, then $L_{A,B}$ is the graph of the self-adjoint operator $-B^{-1}A$. Thus, the Lagrangian subspaces can be considered a compactification of the set of self-adjoint operators.

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Note the the correspondence between unitary U and self-adjoint $-B^{-1}A = i(I+\tilde{U})^{-1}(I-\tilde{U})$ is the Cayley transform that is sometimes used to study unbounded self-adjoint operators.

Now we discuss the process of symplectic reduction. Let G be a co-isotropic subspace of $X \oplus X$. Then $G^\omega \subseteq G$ is isotropic and the quotient G/G^ω is again a symplectic space with symplectic form

$$\overline{\omega}[z + G^\omega, w + G^\omega] = \omega[z, w]$$

If L is a Lagrangian subspace of $X \oplus X$ then $\overline{L} = \pi(L \cap G)$ is Lagrangian in G/G^ω. Here π denotes the projection onto the quotient space. In the presence of an inner product we can identify G/G^ω with the orthogonal complement of G^ω in G. We may also identify Lagrangian subspaces of G/G^ω with Lagrangian subspaces L of $X \oplus X$ satisfying $G^\omega \subseteq L \subseteq G$.

To get an explict formula for $\overline{L_U}$ we digress to give a description of co-isotropic subspaces and their isotropic skew complements. These are parametrized by partial isometries from $K_+ \to K_-$. Let V be such a partial isomtery with initial space $K_{+,0} \subseteq K_+$ and final space $K_{-,0} \subseteq K_-$. Make orthogonal decompositions $K_+ = K_{+,0} \oplus K_{+,1}$ and $K_- = K_{-,0} \oplus K_{-,1}$. Then V is unitary from $K_{+,0} \to K_{-,0}$ and the associated co-isotropic subspace is

$$G_V = \{z_{+,0} + z_{+,1} + z_{-,0} + z_{-,1} : z_{-,0} = V z_{+,0}\}$$

The skew complement is

$$G_V^\omega = \{z_{+,0} + z_{+,1} + z_{-,0} + z_{-,1} : z_{-,0} = V z_{+,0} \text{ and } z_{+,1} = z_{-,1} = 0\}$$

and

$$G_V / G_V^\omega = K_{+,1} \oplus K_{0,1}$$

with $\overline{J}$ given by $iI \oplus -iI$.

Now let L_U be the Lagrangian associated with the unitary U. Write U in block form $\begin{bmatrix} U_{0,0} & U_{0,1} \\ U_{1,0} & U_{1,1} \end{bmatrix}$ with respect to the orthogonal decomposistions of $K\pm$ above.

Proposition 1.3

$$\overline{L_U} = L_{\overline{U}}$$

where

$$\overline{U} = U_{1,1} + U_{1,0}(V - U_{0,0})^{-1}U_{0,1}$$

Graphs with boundary and Laplacians with boundary conditions

We now wish to consider the discrete analogues of Dirichlet and Neumann Laplacians on a graph with boundary. In fact, one can produce a discrete version of the theory of self-adjoint

extensions of symmetric operators [CdV, KS]. Here we concentrate on extensions of the Laplacian Δ (we drop the γ subscript).

A graph with boundary is a graph with a distinguished subset V_b of vertices called boundary vertices. The set of interior vertices V_i is the complement $V_i = V \setminus V_b$.

We may decompose $\ell^2(V) = \ell^2(V_i) \oplus \ell^2(V_b)$. Let P and Q be the corresponding orthogonal projections. For $u \in \ell^2(V)$, the boundary value of u is Qu, while the discrete analogue of the normal derivative is $Q\Delta u$.

We begin with the Lagrangian subspace

$$\text{Graph}(\Delta) \subset \ell^2(V) \oplus \ell^2(V)$$

and consider the projection

$$G = P \oplus P(\text{Graph}(\Delta)) = \left\{ \begin{bmatrix} Pu \\ P\Delta u \end{bmatrix} : u \in \ell^2(V) \right\}.$$

The subspace G is co-isotropic in $\ell^2(V_i) \oplus \ell^2(V_i)$, but not Lagrangian. This would require

$$\langle Pu, P\Delta u \rangle - \langle P\Delta u, Pu \rangle = \langle u, P\Delta u \rangle - \langle P\Delta u, u \rangle = 0$$

for every $u \in \ell^2(V)$, but $P\Delta$ is not self-adjoint. A calculation shows that the skew complement of G is

$$G^\omega = \left\{ \begin{bmatrix} Pu \\ P\Delta Pu \end{bmatrix} : u \in \ell^2(V) \text{ with } Q\Delta u = 0 \right\}$$

which implies that $G^\omega \subset G$.

Definition: A *self-adjoint extension* of Δ is a self-adjoint operator on $\ell^2(V_i)$ whose graph is a Lagrangian L with $G^\omega \subset L \subset G$.

Thus if the Lagrangian L satisfies $G^\omega \subset L \subset G$, and is a graph, then every $\begin{bmatrix} Pu \\ P\Delta u \end{bmatrix} \in L$ is of the form $\begin{bmatrix} Pu \\ \Delta_L Pu \end{bmatrix}$ for the self-adjoint extension Δ_L associated with L. The set of all Lagrangians with $G^\omega \subset L \subset G$ is a compactification of the set of self-adjoint extensions. Notice that this set of Lagrangians can be identified with the set of all Lagrangian subspaces of the symplectic reduction $\overline{G} = G/G^\omega$.

Notice that both G and G^ω have the form

$$G_D = \left\{ \begin{bmatrix} Pu \\ P\Delta u \end{bmatrix} : u \in D \right\} \tag{1.4}$$

for a subspace $D \subseteq \ell^2(V)$, which we call the domain. For G we have $D = \ell^2(V)$ while for G^ω we have $D = D_0 = \{ u \in \ell^2(V) : Qu = Q\Delta u = 0 \}$. In the second case, the elements of D obey both Dirichlet and Neumann boundary conditions, while in the first case they don't obey any boundary conditions at all.

It is fairly easy to see that the Lagrangians L corresponding to self-adjoint extensions must also be of the form G_D for some domain D with $D_0 \subset D \subset \ell^2(V)$. However, D is not unique, since we may add u with $Pu = P\Delta u = 0$ to D without changing G_D.

Now we consider the projection

$$F = Q \oplus Q(\mathrm{Graph}(\Delta)) = \left\{ \begin{bmatrix} Qu \\ Q\Delta u \end{bmatrix} : u \in \ell^2(V) \right\}.$$

Elements of F are the possible boundary values in $\ell^2(V_b) \oplus \ell^2(V_b)$. As was the case with G, F is co-isotropic and we may consider the symplectic reduction F/F^ω.

Proposition 1.4 *The spaces G/G^ω and F/F^ω are symplectically isomorphic*

Proof: First we define a map from G onto F/F^ω. Let $z \in G$. Then $z = \begin{bmatrix} Pu \\ P\Delta u \end{bmatrix}$ for some $u \in \ell^2(V)$.
Consider $z' = \begin{bmatrix} Qu \\ Q\Delta u \end{bmatrix} \in F$. Then the equivalence class $\pi(z') \in \overline{F} = F/F^\omega$ does not depend on u.
For suppose that

$$z = \begin{bmatrix} Pu_1 \\ P\Delta u_1 \end{bmatrix} = \begin{bmatrix} Pu_2 \\ P\Delta u_2 \end{bmatrix}$$

Then $P(u_1 - u_2) = 0$ and $P\Delta(u_1 - u_2) = 0$. Now let $z' = \begin{bmatrix} Qu_1 \\ Q\Delta u_1 \end{bmatrix}$ and $z'' = \begin{bmatrix} Qu_2 \\ Q\Delta u_2 \end{bmatrix}$. Then for any $v \in \ell^2(V)$

$$\omega \left[\begin{bmatrix} Q(u_1 - u_2) \\ Q\Delta(u_1 - u_2) \end{bmatrix}, \begin{bmatrix} Qv \\ Q\Delta v \end{bmatrix} \right]$$

$$= \langle Q(u_1 - u_2), Q\Delta v \rangle - \langle Q\Delta(u_1 - u_2), Qv \rangle$$

$$= \langle Q(u_1 - u_2), \Delta v \rangle - \langle Q\Delta(u_1 - u_2), v \rangle$$

$$= \langle Q(u_1 - u_2) + P(u_1 - u_2), \Delta v \rangle - \langle Q\Delta(u_1 - u_2) + P\Delta(u_1 - u_2), v \rangle$$

$$= \langle (u_1 - u_2), \Delta v \rangle - \langle \Delta(u_1 - u_2), v \rangle = 0$$

Thus $\begin{bmatrix} Q(u_1 - u_2) \\ Q\Delta(u_1 - u_2) \end{bmatrix} \in F^\omega$ which implies that $\pi(z') = \pi(z'')$
Thus map sending $z \mapsto \pi(z')$ is well defined.

$$\vdots$$

$\square$

Now we see that self-adjoint extensions are parametrized by Lagrangian subspaces of F/F^ω, and so by the unitary group of dimension $\dim(F/F^\omega)/2$.

Formula for the self-adjoint extensions

We wish to obtain a formula for the self-adjoint extension of the Laplacians. The idea is that for $u \in D$ we have that $\Delta_U P u = P \Delta u$, where Δ_U is the self-adjoint extension. So, beginning with $v \in \ell^2(V_i)$, i.e., $Pv = v$, we first find try to find $w \in \ell^2(V_b)$ such that $v + w$ is in the domain. Then $\Delta_U v = \Delta_U P(v + w) = P\Delta(v + w)$.

For $v + w$ to be in D, it must satisfy the boundary conditions. Thus we must have

$$\Big(I + U + i(I - U)Q\Delta Q\Big)w = -i(I - U)Q\Delta Pv.$$

Proceeding formally (i.e., assuming that $I + U + i(I - U)Q\Delta Q$ is invertible), we obtain

$$w = -i\Big(I + U + i(I - U)Q\Delta Q\Big)^{-1}(I - U)Q\Delta Pv$$

so that
$$\Delta_U = P\Delta P - iP\Delta Q\Big(I + U + i(I - U)Q\Delta Q\Big)^{-1}(I - U)Q\Delta P$$

$$= P\Delta P - P\Delta Q\Big(-i(I - U)^{-1}(I + U) + Q\Delta Q\Big)^{-1}Q\Delta P$$

The case $U = I$ corresponds to Dirichlet boundary conditions. So the Dirichlet Laplacian is

$$L_I = P\Delta P.$$

The case $U = -I$ corresponds to Neumann boundary conditions. So the Neumann Laplacian is

$$\Delta_{-I} = P\Delta P - P\Delta Q\Big(Q\Delta Q\Big)^{-1}Q\Delta P$$

(Straigten out what happens when things are not invertible. Notice that there shouldn't be an answer if G_D is not a graph.)

Self-adjoint boundary conditions

We will call a homogeneous boundary condition on $u \in \ell^2(V)$ of the form

$$AQu + BQ\Delta u = f$$

a self-adjoint boundary condition if A, B define a Lagrangian subspace, i.e., AB^* is self-adjoint and $\begin{bmatrix} A & B \end{bmatrix}$ has maximal rank. Note that the kernel of the map $u \to AQu + BQ\Delta u$ is exactly $L_{A,B}$, so giving a boundary condition is the same as specfying the equivalence class of $\begin{bmatrix} Qu \\ Q\Delta u \end{bmatrix}$ in $\ell^2(V_b) \oplus \ell^2(V_b)/L_{A,B}$. In the presence of an inner product, we may identify $\ell^2(V_b) \oplus \ell^2(V_b)/L^{A,B}$ with $L_{A,B}^{\perp}$.

If we switch now to the description in terms of unitary operators, we find $L_U^{\perp} = L_{-U}$ and we can write a boundary condition in the form

$$\mathrm{Proj}_{L_{-U}} \begin{bmatrix} Qu \\ Q\Delta u \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$

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Formula for $\begin{bmatrix} a \\ b \end{bmatrix}$ in terms of f ...

Solving boundary value problems

We now discuss solutions to the boundary value problem

$$(P - \lambda)\Delta u = 0$$

$$AQu + BQ\Delta u = f$$

or, equivalently

$$(P - \lambda)\Delta u = 0$$

$$\mathrm{Proj}_{L-U} \begin{bmatrix} Qu \\ Q\Delta u \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$

Proposition 1.5 *If $\Delta_U - \lambda$ is invertible, then the boundary value problem has a solution*