Hermitian Operators and Boundary Conditions

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1 Hermitian Operator Definition

An operator is Hermitian if $A^* = A$. Recall that we define the adjoint via the inner product: $(Ax, y) = (x, A^* y)$ for all x, y. If we were dealing with matrices, then $(Ax, y) = (Ax)^T y = x^T A^T y$ so $A^* = A^T$. So in some sense, when we are thinking about PDEs, A^* is a generalization of the transpose to infinite matrices. A Hermitian operator is one which is then invariant under transpose. We have recently seen two infinite matrices which satisfy this property. The discretization of the Laplace in terms of Fourier modes:

$$\Delta = \begin{bmatrix} -(\pi)^2 & 0 & 0 \\ 0 & -(2\pi)^2 & \ddots \\ 0 & \ddots & \ddots \end{bmatrix} = D$$

and the finite difference discretization of the Laplacian:

$$\delta_0^2 = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \end{pmatrix}$$

are both matrices that can flip rows and columns and have the same structure (except we need to be careful at the boundaries for δ_0^2, a point we will go into more detail with later). It might not surprise you that the Laplacian is self-adjoint (under the right boundary conditions). The way we prove it in the general case is by directly dealing with the integral. Recall that

$$\begin{aligned}(\Delta f, g) &= \int_\Omega \Delta f(x) g(x) dx \\ &= |f''(x)g(x)|_0^1 - \int_\Omega f'(x)g'(x)dx \\ &= |f''(x)g(x)|_0^1 - |f(x)g''(x)|_0^1 + \int_\Omega f(x)\Delta g(x)dx \\ &= |f''(x)g(x)|_0^1 - |f(x)g''(x)|_0^1 + (f, \Delta g)\end{aligned}$$

So whether Δ is self-adjoint does depend on what happens at the endpoints. This is what we call boundary conditions and is just the beginning of our emphasis on their importance. So one way for Δ to be self-adjoint is to be in the space where $f(0) = f(1) = 0$, in which case all of the boundary terms are zero. Or we can simply have periodic conditions, where $f(0) = f(1)$. This is why the Fourier basis is so natural!

2 Boundary Conditions

2.1 Investigating a Few

But handling the boundary conditions points out that we need to be careful about our operator discretizations. Notice that the first term in the stencil matrix is really $u(0) - 2u(\Delta x) + u(2\Delta x)$. At this point, we need to know something about $u(0)$ order to write the first line. This means to that the PDE is actually only solved on the interior of the domain, since the boundary conditions then give what the value at the boundaries will be. If $u(0) = u(1) = 0$, then that's the same as chopping off the last terms of the stencil and so we get:

$$\delta_0^2 = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & -2 \end{pmatrix}$$

if $u'(0) = u'(1) = 0$, then we have the equation $u(0) - 2u(\Delta x) + u(2\Delta x)$ at the end, but we can get $u(0)$ through a derivative approximation:

$$u'(0) \approx \frac{u(2\Delta x) - u(0)}{2\Delta x}$$

which implies a first order approximation of $u(2\Delta x) = u(0)$, and so we get the stencil:

$$\delta_0^2 = \begin{pmatrix} -2 & 2 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 2 & -2 \end{pmatrix}$$

If we have periodic boundary conditions $u(0) = u(1)$, we would instead take the $u(i\Delta x)$ with $i = 0$ at the start, and then the wrap-around would give

$$\delta_0^2 = \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ 1 & & & 1 & -2 \end{pmatrix}$$

(losing the bandedness!).

2.2 Problem

What happens if $u(0) = u(1) = a > 0$? Then we would have at the end $a - 2u(\Delta x) + u(2\Delta x)$. How can you express this in a linear operator? The issue is... you can't! With these boundary conditions the finite difference stencils now become affine, i.e. $ax + b$ instead of simply ax.

2.3 Boundary Conditions, Function Spaces, and Extrapolation

These issues with boundary conditions requires us to get a little more formal with our handling of the PDE. Take the Heat Equation $u_t = \Delta u$ defined on some domain Ω. For example, $\Omega = (0, 1)$. The boundary conditions are some conditions on $u(x)$ for $x \in \partial\Omega$. The derivative operator goes from u defined on $\overline{\Omega}$ to a value defined in Ω. i.e. the derivative operator changes the "type" of the function or the "space" it lives in. That isn't too hard to think about though: we take two derivatives, so if the function was twice-differentiable, now it's something not differentiable. So there is a difference in the properties of u after Δ is applied.

Now let's think of the PDE with a bit more formalism. Since the boundaries are fixed, if u is defined on Ω, we want to write our PDE in the interior Ω. Let Q be the operator that "extends" u to the boundary condition. Then we have that

$$u_t = \Delta Q u$$

in Ω. What this is saying is that, we need to take u to a space where it is defined on $\overline{\Omega}$ before we apply the Laplacian. That extension to the boundary is equivalent to the boundary condition. For example, if we say that Q extends to the boundary by $u(0) = u(\Delta x)$, then Q is saying that $u'(0) = 0$ in a first order approximation. But $Q = (Q_L, Q_b)$ can be affine, where $Qu = Q_L u + b$. For example, with $u(0) = 5$ as a boundary condition, we take the interior u and then attach a 5 on the end to get the coefficients which include the boundary. In this form, the Laplacian is always discretized as an $N \times (N + 2)$ matrix:

$$\delta_0^2 = \begin{pmatrix} 1 & -2 & 1 & & & \\ 0 & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \end{pmatrix}$$

since now the boundary values are the first and last values of the U array in the approximation. Notice then that the composition of the two operators, ΔQ, is an $N \times N$ system that maps u on the interior back to u on the interior. This approach then directly generalizes to having more difficult boundary conditions.