Physics 605: Solving 2D linear partial differential equations Due: never

1 The diffusion equation

We are going to start by considering a simple partial differential equation, the diffusion equation:

$$\frac{\partial u(x,t)}{\partial t} = D \frac{\partial^2 u}{\partial t^2}.$$
(1)

Such an equation is used to describe the diffusion of particles in a fluid (where u is the number density of particles) or the transport of heat through a material (there it is usually called the heat equation and u is the temperature). Our job will be to show that solving such an equation is helped by the vector space apparatus we've developed. Before we get to the math, we need to deal with some physics associated with this equation. Suppose the domain of x is between 0 and L. Integrate both sides of Eq. (1) within that domain to find

$$\frac{\partial}{\partial t} \int_0^L dx \ u(x,t) = D \frac{\partial u(x,t)}{\partial x} \Big|_0^L.$$
(2)

Using the interpretation of Eq. (1) as describing the diffusion of particles, we see that the left hand side gives the change in time of the total number of particles. The right hand side, on the other hand, tells you that the total number of particles can change if and only if

$$J = D \frac{\partial u(x,t)}{\partial t} \Big|_{0,L} \neq 0, \tag{3}$$

on at least one boundary. We interpret J as the flux of particles escaping through one or the other boundary. Therefore, we expect J = 0 on the boundary. This gives us a **boundary condition**,

$$D\frac{\partial u(x,t)}{\partial t}\Big|_{0,L} = 0.$$
(4)

We want to solve the diffusion equation subject to this boundary condition on both boundaries.

Consider the set of functions in x such that $\partial f(x)/\partial x = 0$ on x = 0 and x = L. This set of functions forms a vector space. Furthermore, consider the

inner product

$$\langle f|g\rangle = \int_0^L dx \ f(x)g(x). \tag{5}$$

Theorem: The operator $\partial^2/\partial x^2$ is self-adjoint.

 $\int_0^L dx f(x) \frac{\partial^2}{\partial x^2} g(x) = -\int_0^L dx \left[\frac{\partial}{\partial x} f(x)\right] \left[\frac{\partial}{\partial x} g(x)\right] = \int_0^L dx \left[\frac{\partial^2}{\partial x^2} f(x)\right] g(x)$ by integrating-by-parts. The integration-by-parts works because $\partial f/\partial x = 0$ for all functions in our vector space so that the boundary term vanishes.

Theorem: The eigenvalues of $\mathcal{L} = \partial^2 / \partial x^2$ are either 0 or negative (non-positive).

To prove this, let $|v\rangle$ be an eigenvector with eigenvalue λ and compute $|v|\mathcal{L}\rangle = \lambda \langle v|v\rangle$. However, note that

$$\langle v | \mathcal{L} v \rangle = -\int_0^L dx \, \left(\frac{\partial v}{\partial x}\right)^2$$
 (6)

after one integration by parts. Therefore, $\lambda \leq 0$.

Now we use the fact a fact that we will not prove: the eigenvectors of a self-adjoint operator in a space of functions with this inner product can form an orthonormal basis for the entire space. Therefore, we want to find the eigenvectors of $\partial^2/\partial x^2$. Let's do that by directly solving the equation:

$$\frac{\partial^2}{\partial x^2}u(x) = -\lambda^2 u(x). \tag{7}$$

Any solution can be written as $u(x) = C_1 \sin(\lambda x) + C_2 \cos(\lambda x)$. To apply the boundary conditions, we note that

$$\frac{\partial u}{\partial x} = \lambda C_1 \cos(\lambda x) - \lambda C_2 \sin(\lambda x). \tag{8}$$

Setting x = 0 and x = +L tells us that

$$C - 1 = 0 \tag{9}$$

$$\lambda C_2 \sin(\lambda L) = 0.$$

We can obviously solve this with $C_1 = C_2 = 0$, but that is just zero. Notice, however, that we can also choose $\lambda = \pi n/L$ for any integer n and $C_1 = 0$ as well. We conclude that there is a set of nontrivial solutions of the form

$$|n\rangle = \frac{1}{\sqrt{L}}\cos\left(\frac{\pi nx}{L}\right).$$
 (10)

These functions are orthonormal (the factor in front is the normalization). Moreover, we found that – with these boundary conditions – we only need $n \ge 0$. And by the theorem we didn't prove, we also know that these functions form a basis for the space of possible functions satisfying our boundary conditions.

Using this result, we notice that any solution $u(x,t) = \sum_{n=0}^{\infty} C_n(t) |n\rangle$. Substituting this into our diffusion equation gives

$$\sum_{n=0}^{\infty} \left[\frac{C_n(t)}{\partial t} + D\left(\frac{\pi n}{L}\right)^2 C_n \right] |n\rangle = 0.$$
 (11)

Since $|n\rangle$ form an orthonormal basis, the coefficients must individually vanish. Therefore,

$$\frac{\partial C_n}{\partial t} + \frac{D\pi^2 n^2}{L^2} C_n = 0.$$
(12)

Therefore, $C_n = \tilde{c}_n e^{-D\pi^2 n^2 t/L^2}$. The most general solution satisfying our boundary conditions is, therefore,

$$u(x,t) = \sum_{n=0}^{\infty} \tilde{c}_n e^{-D\pi^2 n^2 t/L^2} \frac{1}{\sqrt{L}} \cos\left(\frac{\pi nx}{L}\right).$$
(13)

Setting t = 0 gives

$$u(x,0) = \sum_{n=0}^{\infty} \tilde{c}_n |n\rangle.$$
(14)

Since this is a basis, we see that we can set the \tilde{c}_n by decomposing the initial condition, u(x, 0) into a linear combination of its eigenfunctions. In particular,

$$\tilde{c}_n = \langle n | u(t=0) \rangle \,. \tag{15}$$

What we just went through is a version of "separation-of-variables." By expanding in eigenfunctions of $\partial^2/\partial x^2$ we were able to separate t and x.

Now let's look at a variant of this problem. Suppose that we have different boundary conditions: $D\partial u/\partial x|_L = J_0$ and $D\partial u/\partial x|_0 = J_0$. In this case we have a constant flux of particles in one side and an equal flux of particles leaving through the other side. Unfortunately, the space of functions satisfying this property is not a vector space. We can, however, write

$$u(x,t) = \frac{J_0}{D}x + \delta u(x,t).$$
(16)

In other words, we have written u as the sum of a solution of $\partial^2 u_0 / \partial x^2 = 0$ satisfying the boundary conditions and a time-dependent δu that still satisfies the diffusion equation,

$$\frac{\partial \delta u}{\partial t} = D \frac{\partial^2 \delta u}{\partial x^2}.$$
(17)

The advantage is that now, δu satisfies boundary conditions such that $\partial \delta u(x,t)/\partial x|_{0,L} = 0$ and the previous analysis applies exactly.

2 Two more PDE examples

2.1 Types of PDEs

PDEs, especially second order ones, can be classified into one of three types. The diffusion equation is the canonical example of the first type, **parabolic**; so is Schrödinger's equation. The other two types of equations are

$$\frac{\partial^2 h}{\partial t^2} - c^2 \frac{\partial^2 h}{\partial x^2} = 0 \qquad \text{hyperbolic}$$
$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \qquad \text{elliptic.}$$

To distinguish them formally, you consider only the highest-order derivative terms. Since most equations we will discuss here are second-order, let's focus on second order equations. Those second-order terms can always be put into the form

$$\sum_{i=1}^{2} \sum_{j=1}^{2} \sigma_{ij} \frac{\partial^2}{\partial x_i \partial x_j} f(x_1, \cdots, x_n).$$
(18)

The matrix whose components are σ_{ij} is called the **symbol** of the differential equation.

Definition: In two dimensions, a PDE is called

$$\begin{array}{ll} \mbox{hyperbolic} & \mbox{det } \sigma < 0 \\ \\ \mbox{parabolic} & \mbox{det } \sigma = 0 \\ \\ \mbox{elliptic} & \mbox{det } \sigma > 0 \end{array}$$

In higher dimensions, the relative signs of the eigenvalues of σ_{ij} determines the character of the equation. If all eigenvalues have the same sign, the equation is **elliptic**, if one eigenvalue has a different sign than the rest then the equation is **hyperbolic** and if one eigenvalue is zero (and the rest have the same sign) the equation is **hyperbolic**. But other situations of a more mixed and complicated character exist.

2.2 The Wave Equation

Consider a string tied at both ends to a wall and under tension. It satisfies the equation

$$\frac{1}{c^2}\frac{\partial^2 h}{\partial t^2} = \frac{\partial^2 h}{\partial x^2}.$$
(19)

This is the wave equation. Again, we will solve it by expanding h(x,t) in eigenfunctions of $\partial^2/\partial x^2$. Note that the vector space of functions we are considering now satisfies the boundary conditions h(L) = 0 and h(0) = 0. Therefore,

$$|n\rangle = \frac{1}{\sqrt{L}}\sin\left(\frac{\pi n}{L}x\right).$$
 (20)

We write

$$h(x,t) = \sum_{n=1}^{\infty} C_n(t) \left| n \right\rangle \tag{21}$$

and derive an equation for the coefficients of $C_n(t)$. These are

$$\frac{\partial^2 C_n}{\partial t^2} = -\frac{c^2 \pi^2 n^2}{L^2} C_n. \tag{22}$$

Consequently, the general solution has the form

$$h(x,t) = \sum_{n=1}^{\infty} \left[\tilde{c}_n \sin\left(c\pi nt/L\right) + \tilde{d}_n \cos\left(c\pi nt/L\right) \right] \frac{1}{\sqrt{L}} \sin\left(\frac{\pi nx}{L}\right).$$
(23)

In this case, there are two coefficients per n, which means that we need two conditions on h(x,0) to fix them. In a typical case, you must provide values for h(x,0) = f(x) and $\partial h(x,t)/\partial t|_{t=0} = v(x)$. Given these choices, we can extract the coefficients to be

$$\tilde{c}_n = \frac{L}{\pi c n} \langle n | v \rangle$$

$$\tilde{d}_n = \langle n | f \rangle .$$

The solution is then

$$h(x,t) = \frac{1}{\sqrt{L}} \sum_{n=1}^{\infty} \left[\langle n|f \rangle \sin(c\pi nt/L) + \frac{L \langle n|v \rangle}{\pi cn} \cos(c\pi nt/L) \right] \sin(\pi nx/L)$$
(24)

in terms of the initial conditions.

2.3 Laplace's equation

Finally consider Laplace's equation, which arises in E&M. This is

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0.$$
 (25)

Let's assume that $\phi(0, y) = \phi(L, y) = 0$. Then we find a general solution

$$\phi(x,y) = \sum_{n=1}^{\infty} \left[\tilde{c}_n \cosh(\pi ny/L) + \tilde{d}_n \sinh(-\pi ny/L) \right] \frac{1}{\sqrt{L}} \sin\left(\frac{\pi nx}{L}\right).$$
(26)

Let's see what happens if we try to solve Laplace's equation using initial conditions. We wish to set

$$\phi(x,0) = f(x), \qquad \frac{\partial \phi}{\partial y}\Big|_{y=0} = g(x)$$
(27)

Then

$$\phi(x,0) = f(x) = \sum_{n=1}^{\infty} \tilde{c}_n \frac{1}{\sqrt{L}} \sin\left(\frac{\pi nx}{L}\right)$$

$$\frac{\partial \phi(x,y)}{\partial y}\Big|_{y=0} = g(x) = -\frac{\pi}{L^{3/2}} \sum_{n=1}^{\infty} n \tilde{d}_n \sin\left(\frac{\pi nx}{L}\right).$$
(28)

Hence,

$$\langle n|f \rangle = \tilde{c}_n$$

 $-\frac{L}{\pi n} \langle n|g \rangle = \tilde{d}_n.$

The solution is

$$\phi(x,y) = \frac{1}{\sqrt{L}} \sum_{n=1}^{\infty} \left[\langle n|f \rangle \cosh(\pi ny/L) + \frac{\langle n|g \rangle L}{\pi n} \sinh(\pi nx/L) \right] \sin(\pi nx/L)$$
(29)

in terms of "initial" conditions at y = 0. Suppose we, instead, try to solve the boundary value problem $\phi(x, 0) = F(x)$ and $\phi(x, L) = G(x)$. Then we have

$$\phi(x,y) = \frac{1}{2\sqrt{L}} \sum_{n=1}^{\infty} \left[\langle n|F+G \rangle \, \frac{\cosh(\pi ny/L)}{\cosh(\pi n)} + \langle n|F-G \rangle \, \frac{\sinh(\pi ny/L)}{\sinh(\pi n)} \right] \sin\left(\frac{\pi nx}{L}\right) \, dx$$

3 Ill-posed problems

Hadamard (in 1902) classified partial differential equation (PDE) problems as being well-posed or ill-posed. A well-posed problem satisfied three conditions:

- 1. There are solutions.
- 2. The solutions are uniquely specified by the boundary conditions.
- 3. The solution's behavior changes continuously with the initial/boundary conditions.

Not all interesting problems are well-posed; not even all interesting problems in physics are well-posed. One example of a well-posed problem is Laplace's equation specified with boundary conditions (these are called **Dirichlet** boundary conditions). Conversely, Laplace's equation also provides us with an example of an ill-posed problem. The solution of Laplace's equation fails to change continuously when initial conditions are specified (the **Cauchy** problem).

The issue can be seen in Eq. (29) when one considers two nearby initial conditions. Lets look, specifically at what happens to the solution at y = L. Then

$$\phi(x,L) = \frac{1}{2\sqrt{L}} \sum_{n=1}^{\infty} \left[\left(\langle n|f \rangle + \frac{\langle n|g \rangle L}{\pi n} \right) e^{\pi n} + \left(\langle n|f \rangle - \frac{\langle n|g \rangle L}{\pi n} \right) e^{-\pi n} \right].$$
(30)

It seems clear that small changes in $\langle n|f\rangle$ and $\langle n|g\rangle$, especially in modes of large n, lead to potentially gigantic changes in $\phi(x, L)$. Indeed, the larger n, the larger the change in $\phi(x, L)$ no matter how small the error in $\langle n|f\rangle$ or $\langle n|g\rangle$ actually is. This mathematical fact prevents us from solving the Cauchy problem for Laplace's equation on a computer – essentially, small errors that occur on the computer aways end up dominating the solutions. In contrast, for the wave equation, there are no exponentials and the solutions tend to be bounded everywhere with respect to the initial conditions.

There is also a class of well-posed problems that are **ill-conditioned**. An error in the initial conditions of an ill-conditioned problem grow as the solution propagates. One can think of the classic case of chaotic trajectories in classical mechanics. For example, two billiard balls with very nearby initial conditions will eventually diverge from each others' paths dramatically even while the balls remain neatly on the table.

4 Characteristics and Hyperbolic Equations

4.1 The wave equation as an example

Hyperbolic equations are special. Consider the wave equation

$$\left[\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2}\right] h(x,t) = 0.$$
(31)

In particular, define

$$2\partial_{\pm} = \frac{\partial}{\partial t} \pm c \frac{\partial}{\partial x}.$$
(32)

Then the wave equation can be rewritten as

$$4\partial_+\partial_-h(x,t) = 0. \tag{33}$$

Indeed, this suggests making a change of variables, $u_{\pm} = x \pm ct$. Then $\partial_{\pm} = \partial/\partial u_{\pm}$.

Rewriting the wave equation, as we did in Eq. (33), shows that all solutions to the wave equation have the following form:

$$h(u_+, u_-) = f(u_+) + g(u_-).$$
(34)

That is, any solution is a sum of an arbitrary function of u_+ and an arbitrary functions of u_- . Or, put another way,

$$h(x,t) = f(x+ct) + g(x-ct).$$
(35)

The lines of constant $x \pm ct$ are called **characteristics** or **characteristic curves**. The existence of characteristics turns out to be a generic feature of hyperbolic differential equations. Often, their solution, or at least the equation, can be simplified dramatically by finding the characteristic curves.

There is a sense in which the characteristics are the lines along which information is propagated by the solutions. If we want to apply initial conditions, h(x,0) and $\partial h(x,t)/\partial t|_{t=0}$ then

$$f(x) + g(x) = h(x, 0)$$

$$c \left[-f'(x) + g'(x) \right] = \frac{\partial h(x, t)}{\partial t} \Big|_{t=0}$$

There is enough information in the functions h(x, 0) and $\partial h(x, t)/\partial t|_{t=0}$ to determine both $f(u_+ \text{ and } g(u_-) \text{ completely.}$ But this need not always be the

case. We might imagine specifies boundary/initial conditions on an entire curve mixing x and t. For example, if we specify h on $u_{+} = 0$ and a derivative of h on $u_{+} = 0$, we will be unable to determine $f(u_{+})$ at all and have too many conditions on $h(u_{-})$.

5 Sturm-Liouville Operator

5.1 General theory

The most general real, self-adjoint, second-order one-dimensional linear operator can be written as

$$\mathcal{L}f = \frac{1}{W(x)} \left[\frac{\partial}{\partial x} \left(p(x) \frac{\partial f}{\partial x} \right) - q(x) f(x) \right]$$
(36)

where W(x) > 0 and p and q are real. This is the **Sturm-Liouville Opera**tor. Many second-order ordinary differential equations in physics occur in this manner. Indeed, let

$$\mathcal{L}' = r(x)\frac{\partial^2}{\partial x^2} + s(x)\frac{\partial}{\partial x} + z(x).$$
(37)

Then **L'** is a Sturm-Liouville operator with $p(x) = \exp\left[\int_a^x d\xi \ s(\xi)/r(\xi)\right], W(x) = p(x)/r(x)$ and q(x) = -z(x)W(x).

This general operator is only self-adjoint under certain boundary conditions and with the inner product $\langle f|g\rangle = \int_a^b dx \ W(x) f^*(x) g(x)$. To see this, compute

$$\langle f|\mathcal{L}g\rangle = p(x)f^*(x)\frac{\partial g}{\partial x}\Big|_a^b - p(x)\frac{\partial f^*(x)}{\partial x}g(x)\Big|_a^b + \langle \mathcal{L}f|g\rangle.$$
(38)

It is self-adjoint so long as the entire expression evaluated at the boundaries vanish (or the functions are periodic in the domain).

Some of the most common, canonical boundary conditions are:

$$f = 0 Dirichlet boundary conditions (39)
 $\frac{\partial f}{\partial r} = 0 Neumann boundary conditions.$$$

There are other ways to satisfy these boundary conditions, however.

The eigenfunctions of $\mathcal{L} \left| f \right\rangle = \lambda \left| f \right\rangle$ give the Sturm-Liouville equation,

$$\frac{\partial}{\partial x} \left[p(x) \frac{\partial f(x)}{\partial x} \right] + q(x) f(x) = \lambda W(x) f(x).$$
(40)

Generically speaking, equations like this are still challenging to solve and historically led to the development of special functions.

5.2 Laplace's equation in polar coordinates

Consider Laplace's equation in polar coordinates,

$$\begin{array}{rcl} x &=& r\cos\theta\\ y &=& r\sin\theta. \end{array}$$

As you can compute readily, Laplace's equation takes the form

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2} = 0 \tag{41}$$

and the inner product in 2D has the form $\langle f|g\rangle = \int dr d\theta r \ f^*(r,\theta)g(r,\theta)$. We can write

$$\phi(r,\theta) = \sum_{m=\infty}^{\infty} c_m(r) e^{im\theta},$$
(42)

using the fact that $e^{im\theta}$ form an orthogonal basis with inner product $\langle f|g\rangle = \int_0^{2\pi} d\theta f^*(\theta)g(\theta)$. Then we have

$$0 = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c_m(r)}{\partial r} \right) - \frac{m^2}{r^2} c_m(r)$$

$$\langle f_m | g_m \rangle = \int_{r_0}^R drr \ f_m^*(r) g_m(r).$$
(43)

This is precisely the form of a Sturm-Liouville problem with W(r) = r, p(r) = rand $q(r) = -m^2/r^2$ – one equation in each sector of m. Note that something strange happens at r = 0; therefore we explicitly write inner and outer bounds on r. We can always make r_0 as small as we want and R as large as we want.

We attempt to solve the equations with $c_m = r^{\alpha}$ for some power α . This gives

$$\left(\alpha^2 - m^2\right)r^{\alpha - 2} = 0,\tag{44}$$

so $\alpha = \pm m$. When m = 0, this only provides one solution. It is easily checked that $c_0 = \ln r$ is also a solution for m = 0, Consequently,

$$\phi(r,\theta) = \sum_{m \neq 0} \left[\tilde{c}_m r^m + \tilde{d}_m r^{-m} \right] e^{im\theta} + \tilde{c}_0 + \tilde{d}_0 \ln r, \tag{45}$$

where the sum over m includes every integer except 0. Are these functions r^{α} orthogonal? No – nor do they have to be. They are all eigenfunctions with zero eigenvalue; there is no theorem that ensures they must be orthogonal.

6 Separation of variables in higher dimensions

Let's now solve Laplace's equation in 3D,

$$\nabla^2 u = 0, \tag{46}$$

in a cubic domain, \mathcal{D} , defined by $0 \leq x, y, z \leq L$.

6.1 Boundary conditions and vector spaces

To choose boundary conditions, we set u(x, y, z) on the boundary of the domain. Let us choose u(x, 0, 0) = u(x, L, 0) = u(x, 0, L) = u(x, L, L) = 0 and u(0, y, z) and u(L, y, z) to be nonzero. With these boundary conditions, we note that ∇^2 is self-adjoint with the inner product

$$\langle f|g\rangle = \int_{\mathcal{D}} dV \ f^*(x, y, z)g(x, y, z) \tag{47}$$

and that the eigenvalues of ∇^2 are always negative (Prove these statements using integration-by-parts).

6.2 "Separation of variables"

We start by choosing one direction, say z, and expanding in eigenfunctions of $\partial^2/\partial z^2$, $\sqrt{2/L}\sin(\pi nx/L) \equiv |n_z\rangle$. Then

$$\phi(x,y,z) = \sum_{n=0}^{\infty} c_n(x,y) \left| n_z \right\rangle = \sum_{n=0}^{\infty} c_n(x,y) \sqrt{\frac{2}{L}} \sin\left(\frac{\pi nz}{L}\right).$$
(48)

This gives us an equation for the coefficients $c_n(x, y)$. This equation is

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]c_n(x,y) - \left(\frac{\pi n}{L}\right)^2c_n(x,y) = 0.$$
(49)

This equation appears to be an eigenfunction equation for the *two-dimensional* Laplacian.

We proceed similarly: choosing y and expanding each $c_n(x, y)$ in a basis of eigenfunctions $c_n(x, y) = \sum_{m=0}^{\infty} d_{nm}(x) |m_y\rangle$ yields

$$\frac{\partial^2 d_{nm}}{\partial x^2} - \left[\left(\frac{\pi m}{L}\right)^2 + \left(\frac{\pi n}{L}\right)^2 \right] d_{nm} = 0.$$
(50)

This equation is an ordinary differential equation which we can solve for each $d_{nm}(x)$. Let $\lambda_{nm}^2 \equiv \left(\frac{\pi m}{L}\right)^2 + \left(\frac{\pi n}{L}\right)^2$. This gives

$$d_{nm}(x) = A_{nm}e^{\lambda_{nm}x} + B_{nm}e^{-\lambda_{nm}x}.$$
(51)

We could have made this decomposition in any combination of the axes and we would, in all cases, obtain a perfectly reasonable formal solution to Laplace's equation. In practice, you should choose the most convenient way to separate variables to solve your problem. Two of the directions will involve an expansion in trigonometric functions and the remaining variable will be solved by exponentials.