MSc Supplementary Course: Mathematical Methods I

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1 Introduction

In this course, we will explore various techniques for solving differential equations, building on basic techniques encountered previously. Of particular interest will be finding ways to solve and understand inhomogeneous linear boundary value problems (BVPs), that is an ordinary differential equation (ODE)

$$Lu(x) = f(x), \quad a < x < b \tag{1}$$

where L is a linear differential operator of the form

$$Lu = a_n u^{(n)}(x) + a_{n-1} u^{(n-1)}(x) + \dots + a_1 u'(x) + a_0 u(x)$$
(2)

and the function f(x) on the right hand side (RHS) is a *forcing function* in the system. Along with equation (1), we impose boundary conditions at x = a and x = b. The number and form of the boundary conditions is essential, and one always thinks of the operator L associated with a particular choice of boundary conditions.

Some questions we will consider:

- 1. How do we solve the system for an arbitrary function f(x)?
- 2. Is there always a solution? If so, is it unique?
- 3. What is the effect of the boundary conditions?
- 4. Can we solve the equation if the $a_k = a_k(x)$ are functions of x?

We remark that the theory of linear BVPs is much richer than the simpler case of linear initial value problems (IVPs) which are often seen in an introductory course on differential equations. In this setting we will primarily use the linear structure of the operator to develop solution techniques which are, in some sense, analogous to finding solutions to matrix equations of the form,

$$\mathbf{A}\vec{x} = \vec{b}.\tag{3}$$

Throughout, we will exploit this analogy to concepts in linear algebra, including the ideas of eigenvectors/eigenvalues, diagonalization, the inverse matrix, etc. Linear differential operators, roughly speaking, can be thought of as infinite-dimensional analogues of linear operators in finite dimensional vector spaces (e.g. matrices), although there are several subtleties in this analogy.

There are numerous applications of developing this theory from estimating energies of quantum systems, to developing spectral methods to solve nonlinear PDEs, to theories of how organisms develop, among many other problems. Additionally, there is a rich theoretical setting (typically taught in courses on Functional Analysis). Here we aim to strike a balance between applications and theory. We will focus on the basic ideas, but will not pursue a fully rigorous treatment, or any particular applications. By the end of the course you should be familiar enough with the ideas to pursue these things at your leisure, and in particular be able to solve specific problems that may arise in the rest of your course.

Material to Review: Broadly speaking this course will use ideas from Linear Algebra to generalize the techniques often seen in courses on Fourier Series or Boundary Value Problems. If you are rusty on these topics please review them now. See the course material for

- Prelims M1: Linear Algebra II
- Prelims: M5: Fourier Series and PDEs.

Further Resources: There are numerous books which cover the general approaches to boundary value problems studied in this course. For example,

- Principles of Applied Mathematics by James Keener (Chapter 1 is review, 2, 4, and 7 cover some material in this course, and other chapters cover material in next term's course);
- The Differential Equations II Reading List also contains many books which cover roughly the same topics (and much more).

1.1 Motivating example: reaction-diffusion equations

The diffusion equation (with or without reactions) is used to model many phenomena. Let u = u(x, t) denote a quantity that depends on one spatial variable x and time t > 0. This could be a chemical concentration, population, density of a substance or even cars in traffic. The diffusion equation can be derived in a very intuitive way: we imagine a segment of space [a, b]. In this segment the total amount of "stuff" is

$$\int_{a}^{b} u(x,t) \, dx. \tag{4}$$

Now, we say that the rate of change of "stuff" in the segment is equal to the amount that leaves/enters through the ends plus any stuff that is added/taken away by the external world. The amount of stuff leaving the ends is the flux, denoted q, and we let f(x, t, u) be a local source function – this is the rate at which u is created or destroyed at position x and time t; note it can in general depend on u itself.



Figure 1: 1D diffusion

The balance is

$$\frac{d}{dt} \int_{a}^{b} u(x,t) \, dx = q(a,t) - q(b,t) + \int_{a}^{b} f(x,t,u) \, dx. \tag{5}$$

This statement should be familiar to you from physics as a *conservation* principle. For instance, if u is a density, then (5) is a statement of conservation of mass. By recognising that

$$q(b,t) - q(a,t) = \int_a^b q_x(x,t) \, dx$$

we obtain

$$\int_{a}^{b} (u_t + q_x - f) \, dx = 0. \tag{6}$$

Equation (6) should hold for any segment and, thus, the integrand must vanish:

$$u_t + q_x = f. \tag{7}$$

To complete the system, the flux needs to be related to the quantity u. A simple relationship is Fick's Law, which states

$$q(x,t) = -Du_x(x,t) \tag{8}$$

where D > 0 is the diffusion constant. Combining (7) and (8), we obtain the diffusion equation

$$u_t - Du_{xx} = f. (9)$$

The classical heat equation is the case f = 0. Many interesting and physically relevant situations are modelled with non-zero f. For example, (9) is a popular model for population dynamics, where f is used to capture growth and other interactions of the population. To seek stationary solutions, we let $u_t = 0$ in (9), and we obtain an equation of the type (1)-(2) albeit a very simple one. Alternatively, we can use separation of variables to construct solutions to the time-dependent problem. In both cases we must solve a BVP in the spatial variables. This is precisely what we will consider in this course. We will sketch an example application in Section 2.9, and use physically-relevant examples as we develop the theory.

2 Eigenfunction methods

Our first approach to solving linear inhomogeneous BVP's is via an eigenfunction expansion. The idea is to exploit the linearity of the operator by constructing a solution as a *superposition* of a (generally infinite) set of functions $\{y_i(x)\}$. In particular, the y_i will be functions satisfying

$$Ly_i(x) = \lambda_i y_i(x), \tag{10}$$

along with homogeneous boundary conditions. Here y_i is an *eigenfunction* with corresponding *eigenvalue* λ_i . This is analogous to the linear algebra eigenproblem

$$\mathbf{A}\vec{x}_i = \lambda_i \vec{x}_i,\tag{11}$$

where **A** is a matrix and \vec{x}_i an eigenvector with eigenvalue λ_i .

2.1 Function spaces

In the same way as linear algebra utilises vector spaces, with linear differential operators we shall think of function spaces. Consider the infinite dimensional space of all reasonably well-behaved functions on the interval $a \le x \le b$.

Similar to a vector space, we can introduce a set of linearly independent basis functions $y_n(x), n = 1, 2, ... \infty$ such that any 'reasonable' function f(x) can be written as a linear combination of these functions:

$$f(x) = \sum_{n=1}^{\infty} c_n y_n(x).$$
(12)

You should have encountered this idea before, with Fourier Series, where the basis functions are sines and cosines; Equation (12) is merely a generalisation. Hence it should be clear that we can have different sets of basis functions.

We also define the **inner product**

$$\langle u, v \rangle = \int_{a}^{b} u(x) \overline{v(x)} \, dx.$$
 (13)

Here the overbar denotes complex conjugate. In this course, we will rarely be concerned with complex valued functions. If it is clear that we are dealing with real functions, we may drop the overbar for simplicity.

2.1.1 Weighting functions

In some instances, the eigenvalue problem and the inner product definition include a weighting function $\rho(x)$, which is required to be real and not change sign on $a \leq x \leq b$. In this case, the relations become

$$Ly_i(x) = \lambda_i \rho(x) y_i(x) \tag{14}$$

and

$$\langle u, v \rangle = \int_{a}^{b} \rho(x) u(x) \overline{v(x)} \, dx.$$
 (15)

2.2 Adjoint

We also require the notion of the *adjoint* of an operator. For operator L with homogenous BC, the adjoint problem $(L^* \text{ BC}^*)$ is defined by the inner product relation

$$\langle Ly, w \rangle = \langle y, L^*w \rangle. \tag{16}$$

To determine the adjoint, one needs to:

- 1. Integrate by parts to move the derivatives of the operator from y to w, and
- 2. Define adjoint boundary conditions so that all boundary terms vanish.

Example

Let $Ly = \frac{d^2y}{dx^2}$ with $a \leq x \leq b$, y(a) = 0 and y'(b) - 3y(b) = 0. We wish to find L^*w , such that $\langle Ly, w \rangle = \langle y, L^*w \rangle$, i.e.,

$$\int_{a}^{b} (y'')(w) \mathrm{d}x = \int_{a}^{b} (y)(L^*w) \mathrm{d}x$$

Solution

We use integration by parts to shift the derivatives from y to w:

$$\int_{a}^{b} wy'' dx = wy'|_{a}^{b} - \int_{a}^{b} w'y' dx$$
$$= wy' - w'y|_{a}^{b} + \int_{a}^{b} yw'' dx$$

The integral gives the formal part so:

$$L^*w = \frac{\mathrm{d}^2w}{\mathrm{d}x^2}.$$

The inner product only includes integral terms, so the boundary terms must vanish. We will exploit this to define boundary conditions on w, i.e. this defines BC^{*}. Here, we require

$$w(b)y'(b) - w'(b)y(b) - w(a)y'(a) + w'(a)y(a) = 0.$$

Using the BC's y'(b) = 3y(b) and y(a) = 0, gives:

$$0 = \left(3w(b) - w'(b)\right)y(b) - w(a)y'(a) + \underbrace{w'(a)y(a)}_{=0}$$

As these terms must vanish for all values of y(b) and y'(a), we infer two BCs on w:

- y(b): 3w(b) w'(b) = 0
- y'(a): w(a) = 0

Definitions

- If $L = L^*$ and $BC = BC^*$, then the problem is *self-adjoint*.
- If $L = L^*$ but $BC \neq BC^*$ we still call the operator self-adjoint.

Aside. Some books use the terminology formally self-adjoint if $L = L^*$ and fully self-adjoint if both $L = L^*$ and $BC = BC^*$.

2.2.1 Eigenfunction Properties

When solving the BVP, the main idea is to construct a solution as a linear combination of eigenfunctions. Two fundamental properties of eigenfunctions will be vital to this approach.

1. Eigenfunctions of the adjoint problem have the same eigenvalues as the original problem

That is,

$$Ly = \lambda y \Rightarrow \exists w \ni L^* w = \lambda w.$$

2. Eigenfunctions corresponding to different eigenvalues are orthogonal

That is, if $Ly_j = \lambda_j y_j$ (so $L^* w_j = \lambda_j w_j$) and $Ly_k = \lambda_k y_k$ ($L^* w_k = \lambda_k w_k$), then for $\lambda_j \neq \lambda_k$, $\langle y_j, w_k \rangle = 0$.

Proof

$$\begin{array}{rcl} \lambda_j \langle y_j, w_k \rangle & = & \langle \lambda_j y_j, w_k \rangle \\ & = & \langle L y_j, w_k \rangle \\ & = & \langle y_j, L^* w_k \rangle \\ & = & \langle y_j, \lambda_k w_k \rangle \\ & = & \lambda_k \langle y_j, w_k \rangle. \end{array}$$

But $\lambda_j \neq \lambda_k$ so $\langle y_j, w_k \rangle = 0$. (The proof is exactly as for matrix problems.)

2.3 Inhomogeneous solution process

We now outline the construction of solutions to the BVP

$$Ly = f(x)$$

with linear, homogeneous, separated boundary conditions, which we denote by $BC_1(a) = 0$ and $BC_2(b) = 0$.

Step 1: Solve the eigenvalue problem

$$Ly = \lambda y, \quad BC_1(a) = 0, \ BC_2(b) = 0$$

to obtain the eigenvalue-eigenfunction pairs (λ_j, y_j) .

Step 2: Solve the adjoint eigenvalue problem

$$L^*w = \lambda w, \quad BC_1^*(a) = 0, \ BC_2^*(b) = 0$$

to obtain (λ_j, w_j) .

Step 3: Assume a solution to the full system Ly = f(x) of the form

$$y = \sum_{i} c_i y_i(x).$$

To determine the coefficients c_i , start from Ly = f and take an inner product with w_k :

$$Ly = f(x)$$

$$\Rightarrow \langle Ly, w_k \rangle = \langle f, w_k \rangle$$

$$\Rightarrow \langle y, L^* w_k \rangle = \langle f, w_k \rangle$$

$$\Rightarrow \langle y, \lambda_k w_k \rangle = \langle f, w_k \rangle$$

$$\Rightarrow \lambda_k \langle \sum_i c_i y_i, w_k \rangle = \langle f, w_k \rangle$$

$$\Rightarrow \lambda_k c_k \langle y_k, w_k \rangle = \langle f, w_k \rangle$$
(17)

We can solve the last equality for the c_k , and we are done! Note that in the last step we have used the orthogonality property $\langle y_j, w_k \rangle = 0$, $j \neq k$.

2.4 Some simple solutions

Note that this construction requires that we can determine the eigenvalues and eigenfunctions. This is by no means guaranteed. We will recall some simple cases, solvable using techniques you should have used before.

• <u>Constant coefficients</u>

$$Ly \equiv ay'' + by' + cy = \lambda y$$

Try $y = e^{mx}$, then:

$$am^2 + bm + (c - \lambda) = 0$$

Then:

- 1. Find roots m_i of the quadratic.
- 2. The general solution is: $y = A_1 e^{m_1 x} + A_2 e^{m_2 x}$. But note there are 3 unknowns: A_1 , A_2 , and λ , while for a second order equation there will only be two BC's.
- 3. Apply first BC to relate A_1 and A_2 .
- 4. Apply second BC to determine values for λ .
- Cauchy-Euler

$$Ly \equiv ax^2y'' + bxy' + cy = \lambda y$$

Try $y = x^m$, then:

$$am(m-1) + bm + (c - \lambda) = 0$$

Then $y = A_1 x^{m_1} + A_2 x^{m_2}$, and repeat the steps above.

2.5 A note on boundary conditions

In the above construction we assumed homogeneous boundary conditions. Consider now the general case of an inhomogeneous system with inhomogeneous boundary conditions,

$$Lu = f(x)$$

$$B_i u = \gamma_i.$$
(18)

A useful technique is to split the system in two, i.e. solve both

$$Lu_1 = f(x), \quad B_i u_1 = 0$$
 (19)

$$Lu_2 = 0, \quad B_i u_2 = \gamma_i. \tag{20}$$

Here, solving for $u_1(x)$ has the difficulty of the forcing function but with zero BC's while the other equation is homogeneous but has non-zero BC's. Due to linearity, it is easy to see that $u(x) = u_1(x) + u_2(x)$ solves the full system (18).

This decomposition can always be performed¹ and since solving (20) tends to be an easier matter (for linear systems!), it is safe for us to focus on techniques for solving the system (19), i.e. homogeneous boundary conditions.

For completeness we note that it is possible to solve BVPs with inhomogeneous BC using an eigenfunction expansion and without performing a decomposition. The key points are:

- 1. The eigenfunctions are *always* determined using homogeneous boundary conditions. Thus, the eigenfunctions will not change whether you "decompose" or not. The difference comes in step 2:
- 2. In going from Line 2 to 3 of (17), care must be taken when performing integration by parts, as boundary terms will generally still be present. (Can you see why?) These extra boundary terms then carry through to the formula for the c_k .

¹As we shall see next term (and you may notice on Problem Sheet 2), it requires caution if there is a zero eigenvalue $\lambda = 0$. We briefly discuss this in Section 2.7.3.

2.6 Connection with linear algebra

There are direct parallels between linear algebra and linear BVPs:

$$\underbrace{\frac{\text{Linear algebra}}{\text{vector } \vec{v} \in \mathbb{R}^n}}_{\text{vector } \vec{v} \in \mathbb{R}^n} \iff \underbrace{\frac{\text{Linear BVP}}{\text{function } y(x) \text{ for } a \leqslant x \leqslant b}}_{\text{function } y(x) \text{ for } a \leqslant x \leqslant b}$$

$$\underbrace{\vec{v} \cdot \vec{w} = \sum_{k=1}^n v_k w_k}_{\text{dot product}} \iff \underbrace{\langle f, g \rangle = \int_a^b f(x) \overline{g(x)} dx}_{\text{inner product}}}_{\text{inner product}}$$

$$\underbrace{\|\vec{v}\|^2 = \vec{v} \cdot \vec{v} \geqslant 0}_{\text{norm}} \iff \underbrace{\|f\|^2 = \langle f, f \rangle \geqslant 0}_{\text{norm}}$$

 $\perp \mbox{ vector } \vec{v} \cdot \vec{w} = 0 \ \ \longleftrightarrow \ \ \mbox{orthogonal function } \langle f,g \rangle = 0$

Matrix $A \iff$ Linear Differential Operator L

Given a vector \vec{v} , the product $A\vec{v}$ is a new vector. Similarly, given a function y(x),

$$Ly = a\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} + b\frac{\mathrm{d}y}{\mathrm{d}x} + cy$$

evaluates to a new function on $a \leq x \leq b$.

In linear algebra, a common problem is to solve the equation

 $A\vec{v}=\vec{b}$

for \vec{v} , given matrix A and vector \vec{b} . Compare that to our general task of solving Ly = f for y, given operator L and RHS f.

Eigenvalue problems

$$\frac{\text{Linear algebra}}{A\vec{v} = \lambda \vec{v}} \xrightarrow{\text{Linear BVP}} Ly = \lambda y$$

How many eigenvalues?

Linear algebra	<u>Linear BVP</u>
A is $n \times n$	L is order n
Solve $ A - \lambda I = 0$	
$\Rightarrow n$ eigenvalues	∞ eigenvalues

Adjoint

	Linear algebra	Linear BVP
	$A \to A^T$	$\begin{array}{c} L \rightarrow L^{*} \\ \mathrm{BC's} \rightarrow \mathrm{BC^{*'s}} \end{array}$
Self adjoint if	$A = A^T$	$L = L^*, BC = BC^*$

A self-adjoint matrix is called Hermitian. A self-adjoint linear differential operator is also referred to as Hermitian. We next look at a particular class of Hermitian operator – Sturm-Liouville operators – that occurs quite commonly and has some useful properties.

2.7 Examples

2.7.1 Homogeneous Boundary Conditions

Suppose we want to solve,

$$Ly = y'' + 3y' + 2y = f(x), \quad y(0) = 0 = y(1).$$
(21)

This has the associated eigenvalue problem

$$Ly = y'' + 3y' + 2y = \lambda y,$$
 (22)

with the same homogeneous Dirichlet conditions. Equation (22) has the characteristic equation,

$$r^2 + 3r + 2 - \lambda = 0 \implies r_{\pm} = \frac{-3 \pm \sqrt{1 + 4\lambda}}{2}.$$
 (23)

We next consider possible values of λ , assuming that it is real.

• If $\lambda > -1/4$, then the solutions are $y = c_1 e^{r \pm t} + c_2 e^{r \mp t}$. Substituting this into the boundary conditions, we have that solutions of this form give the following linear system for the constants,

$$\begin{pmatrix} 1 & 1\\ e^{r_{\pm}} & e^{r_{\mp}} \end{pmatrix} \begin{pmatrix} c_1\\ c_2 \end{pmatrix} = \begin{pmatrix} 0\\ 0 \end{pmatrix}.$$
 (24)

We see that the determinant of this system is never zero, and hence we must have $c_1 = c_2 = 0$.

- If $\lambda = -1/4$, then the solutions for the homogeneous problem are $y = e^{-\frac{3x}{2}} (c_1 + c_2 x)$. The boundary condition y(0)=0 requires $c_1 = 0$, and then the boundary condition y(1) = 0 will force $c_2 = 0$, so this is not an eigenvalue either.
- If $\lambda < -1/4$, then we have a complex-conjugate pair of solutions to (23), so solutions take the form

$$y = e^{-\frac{3x}{2}} \left(c_1 \cos(\omega x) + c_2 \sin(\omega x) \right)$$

where

$$-\omega^2 = \frac{1+4\lambda}{4}$$

The boundary condition y(0) = 0 will force $c_1 = 0$. The condition y(1) = 0 then requires $\sin(\omega) = 0$, so that $\omega = n\pi$ for an integer n. Hence the eigenvalues are of the form $\lambda = -\frac{1}{4} - (n\pi)^2$ for $n = 1, 2, 3, \ldots$

In order to use the eigenfunction theory, we have to study the adjoint operator. Doing the integration by parts, we find the adjoint eigenvalue problem of the form,

$$L^*w = w'' - 3w' + 2w = \lambda w. \quad w(0) = 0 = w(1).$$
(25)

We already know the eigenvalues λ , and so we in fact know these eigenfunctions immediately. After using the boundary conditions, they are

$$w = e^{\frac{3x}{2}}\sin(\omega x)$$

where ω is as before.

Exercise: Follow the same procedure for the BVP,

$$Ly = x^{2}y'' + xy' = f(x), \quad y(1) = 0 = y(2).$$
(26)

What are the eigenfunctions? Adjoint eigenfunctions? Eigenvalues? Finally, how can you solve the problem given an arbitrary forcing function f(x)?

2.7.2 Inhomogeneous Boundary Conditions

Let y'' = f(x) with $0 \le x \le 1$, $y(0) = \alpha$ and $y(1) = \beta$. Then:

BC's Incorporated Solution Route

1. Solve $y'' = \lambda y$, with y(0) = 0 and y(1) = 0.

We get $y_k(x) = \sin(k\pi x)$ and $\lambda_k = -k^2\pi^2$ with $k = 1, 2, 3, \dots$

The problem is self-adjoint (show this as an exercise), so $w_k = y_k = \sin(k\pi x)$ and $w''_k = -\lambda_k w_k$ where $\lambda_k = -k^2 \pi^2$.



$$y'' = f(x)$$
$$\int_{0}^{1} w_{k} y'' dx = \int_{0}^{1} w_{k} f dx$$
$$\Rightarrow (y'w_{k} - yw'_{k})|_{0}^{1} + \int_{0}^{1} w''_{k} y dx = \int_{0}^{1} w_{k} f dx$$
$$\Rightarrow (y'w_{k} - yw'_{k})|_{0}^{1} + \lambda_{k} \int_{0}^{1} w_{k} y dx = \int_{0}^{1} w_{k} f dx$$
$$\Rightarrow (y'w_{k} - yw'_{k})|_{0}^{1} + \lambda_{k} c_{k} \int_{0}^{1} w_{k} y_{k} dx = \int_{0}^{1} w_{k} f dx$$
$$\Rightarrow (y'w_{k} - yw'_{k})|_{0}^{1} - k^{2}\pi^{2}c_{k} \int_{0}^{1} \sin^{2}(k\pi x) dx = \int_{0}^{1} w_{k} f dx$$

3. Now $\int_0^1 \sin^2(k\pi x) \, dx = 1/2$, and $w_k = \sin(k\pi x)$, hence

$$\begin{aligned} y'w_k - yw'_k|_0^1 &= -k\pi\cos(k\pi)y(1) + k\pi\cos(0)y(0) \\ \Rightarrow -\beta k\pi(-1)^k + \alpha k\pi - \frac{1}{2}k^2\pi^2 c_k &= \int_0^1 f(x)\sin k\pi x dx \\ \Rightarrow c_k &= -\frac{2\int_0^1 f(x)\sin(k\pi x) dx}{k^2\pi^2} + \frac{2}{k\pi} \left(\alpha - (-1)^k\beta\right). \end{aligned}$$

Solving for c_k gives y(x) as a Fourier series.

Decomposed Solution Route

1. Solve two systems separately:

$$y'' = f(x), \quad y(0) = y(1) = 0$$

 $u'' = 0, \quad u(0) = \alpha, \ u(1) = \beta$

2. To solve for y, since BC=0 we can jump straight to the formula

$$\hat{c}_k = -\frac{\langle f, w_k \rangle}{\lambda_k \langle y_k, w_k \rangle} = -\frac{2\int_0^1 f(x) \sin(k\pi x) \, dx}{k^2 \pi^2}.$$

3. The solution for u is easily obtained as

$$u = (\beta - \alpha)x + \alpha$$

4. The full solution is y(x) + u(x).

Although they look different, both approaches give the same solution. Either way, we see that self-adjoint problems are great: they are less work since the w_k 's are the same as the y_k 's.

2.7.3 Zero Eigenvalues

We will cover the following in more detail next term, but let's go through the case with zero eigenvalues so you can clearly see why these issues arise. Consider the boundary value problem,

$$y'' = f(x), \quad y'(0) = 0, \quad y'(1) = 0.$$
 (27)

You should confirm that this is a fully self-adjoint operator and that it has the eigenfunctions and eigenvalues,

$$y_n = \cos(n\pi x), \quad \lambda_n = -(n\pi)^2, \quad n = 0, 1, 2, \dots$$

For n = 0, y_0 is a constant function (without loss of generality, we could take $y_0 = 1$, for instance). Note that you can find this eigenfunction directly by solving Ly = 0, and if any solutions satisfy the boundary conditions, then the operator automatically has a zero eigenvalue.

If we follow the procedure in Section 2.3 for any eigenfunction with $n \ge 1$, everything works as intended and we can find the corresponding c_n 's. However, when n = 0, we see that $\langle y, Ly_0 \rangle = 0$. So, the last line of the derivation in (17) reads $0 = \langle f, y_0 \rangle$. As we will show next term, this means that solutions only exist if this condition is satisfied. In this case, any solution to (27) is also not unique as if y is such a solution, then so is $y + \alpha y_0$ for any constant $\alpha \in \mathbb{R}$. If instead $\langle f, y_0 \rangle \neq 0$, then the boundary value problem does not have a solution.

Example.

Let f(x) = 1 in problem (27) and let's try solving the BVP directly. Integrating (27) twice we get $y = x^2/2 + Bx + C$. Applying y'(0) = 0 we have B = 0, but we then see $y'(1) = 1 \neq 0$, for any choice of the constant C, and so there are no solutions to this problem. If instead we let f(x) = 0, we see that any constant satisfies this equation and boundary conditions, as predicted above.

Note: in general, in particular if the operator is not self-adjoint, the situation is as follows. Consider the problem Ly = f(x), the associated eigenvalue problem $Ly = \lambda y$, and adjoint eigenvalue problem $L^*w = \lambda w$. If there is a zero eigenvalue, then one of the following is true:

(i) if $\langle f, w_0 \rangle \neq 0$, then the problem has no solution for this f(x), or, (ii) if $\langle f, w_0 \rangle = 0$, then the problem has infinitely many solutions, given by

adding multiples of the associated eigenvector, y_0 , to the solution.

There are two technical issues we did not address here. First, how do we know that an arbitrary function y can be expressed as a sum of eigenfunctions? Secondly, how do we know to only look for real eigenvalues λ ? The first question is in general a difficult one that requires some machinery of Functional Analysis, so we will simply assume that the eigenfunctions form a complete set - general Theorems will guarantee this for a wide class of problems of the form we have studied. The second question can be answered via Sturm-Liouville theory, which we address in the next subsection.

2.8 Sturm-Liouville theory

Sturm–Liouville (SL) theory of second order concerns eigenvalue problems of the form:

$$Ly = \lambda r(x)y$$

where $r(x) \ge 0$ is a weighting function, and the operator L is of the form

$$Ly = -\frac{\mathrm{d}}{\mathrm{d}x} \left(p(x) \frac{\mathrm{d}y}{\mathrm{d}x} \right) + q(x)y, \ a \le x \le b$$
(28)

The functions p, q, and r are all assumed to be real. It is easy to check that the operator is formally self-adjoint. It is *fully self-adjoint* if the boundary conditions take the separated form

$$\alpha_1 y(a) + \alpha_2 y'(a) = 0$$

$$\alpha_3 y(b) + \alpha_4 y'(b) = 0.$$

Observe also that if p(a) = p(b) = 0, then $\langle Ly, w \rangle = \langle y, Lw \rangle$ irrespective of boundary conditions. This defines the so-called natural interval [a, b] for the problem. We will always assume that p(x) does not change sign in the interval [a, b].

2.8.1 Inhomogeneous SL problems

Since a SL operator is self-adjoint, the eigenfunction expansion process is straightforward. Consider

$$Ly = f(x)$$

with homogeneous BC's. The system can be solved with an eigenfunction expansion in the same manner as in Section 2.3.

Let's assume that $y = \sum_j c_j y_j$ and note that $\langle j, Ly_k \rangle = 0$ if $j \neq k$. Then, it is straightforward to deduce the following:

$$Ly = f(x)$$

$$\Rightarrow \langle Ly, y_k \rangle = \langle f, y_k \rangle$$

$$\Rightarrow \langle y, Ly_k \rangle = \langle f, y_k \rangle \quad (\text{since } L^* = L, \text{ and } w_k = y_k) \quad (29)$$

$$\Rightarrow \langle y, \lambda_k ry_k \rangle = \langle f, y_k \rangle$$

$$\Rightarrow \lambda_k c_k \langle y_k, ry_k \rangle = \langle f, y_k \rangle,$$

Thus we obtain the formula

$$c_k = \frac{\langle f, y_k \rangle}{\lambda_k \langle y_k, ry_k \rangle} \tag{30}$$

and the full solution is given by

$$y = \sum_{k} c_k y_k.$$

2.8.2 Transforming an operator to SL form

Many problems encountered in physical systems are Sturm-Liouville. In fact, any operator

$$Ly \equiv a_2(x)y''(x) + a_1(x)y'(x) + a_0(x)y(x)$$

with $a_2(x) \neq 0$ in the interval can be converted to a SL operator. To *transform* to a self-adjoint SL operator, multiply by an integrating factor function $\mu(x)$:

$$\mu a_2 y'' + \mu a_1 y' + \mu a_0 y$$

We then choose μ so that the first and second derivatives collapse, i.e. so it can be expressed in the form

$$-\frac{d}{dx}(py') + qy$$

Suppose we are considering the problem

$$Ly = f(x)$$

where L is not Sturm-Liouville. We could solve following the approach in equation (17); alternatively we could convert to Sturm-Liouville first, and then proceed using the nice properties of a self-adjoint operator. So, is the problem self-adjoint or isn't it?? The key observation is that we are no longer solving the same problem. We have transformed to a new operator

$$\hat{L}y = -\frac{d}{dx}(py') + qy$$

which does not satisfy the same equation as the original, that is Ly = f while $\hat{L}y = \mu f$. They are both valid, and must ultimately lead to the same solution.

2.8.3 Further properties

Orthogonality.

Due to the presence of the weighting function, the *orthogonality* relation is

$$\int_{a}^{b} y_k(x) y_j(x) r(x) \mathrm{d}x = 0.$$
(31)

Eigenvalues.

The functions p, q, r are real, so $\overline{L} = L$. Thus, taking the conjugate of both sides of $Ly_k = \lambda_k y_k$ gives

$$L \ \overline{y_k} = \overline{\lambda_k} \ r \ \overline{y_k}$$

$$\Rightarrow \langle y_k, L \ \overline{y_k} \rangle = \overline{\lambda_k} \langle y_k, r \ \overline{y_k} \rangle$$
(32)

but

Thus, all eigenvalues are real.

If $a \leq x \leq b$ is a finite domain, then λ 's are discrete and countable: $\lambda_1 < \lambda_2 < \lambda_3 < \cdots < \lambda_k < \cdots$, with $\lim_{k \to \infty} \lambda_k = \infty$.

Eigenfunctions.

The $\{y_k\}$ are a *complete set*, that is all h(x) with $\int h^2 r \, dx < \infty$ can be expanded as

$$h(x) = \sum c_k y_k(x).$$

Take an inner product with $r(x)y_j(x)$:

$$\langle ry_j, h \rangle = \langle ry_j, \sum c_k y_k \rangle = \sum c_k \langle ry_j, y_k \rangle = c_j \langle ry_j, y_j \rangle$$

$$\Rightarrow c_j = \frac{\int_a^b h(x) y_j(x) r(x) \, dx}{\int_a^b y_j^2(x) r(x) \, dx}$$

Note: We've used h(x) to make clear that we're not talking about the solution to the BVP; rather, we are expanding any function that is suitably bounded on the same domain.

2.8.4 Other tidbits

Regular Sturm-Liouville Problems. If the system satisfies all of the above and the additional conditions

- p(x) > 0 and r(x) > 0 on $a \le x \le b$.
- $q(x) \ge 0$ on $a \le x \le b$.
- BCs have $\alpha_1 \alpha_2 \leq 0$ and $\alpha_3 \alpha_4 \geq 0$,

then $\lambda_k \ge 0$ for $k = 1, 2, 3, \ldots$.

Proof: Using $\langle y_k, Ly_k - \lambda_k r y_k \rangle = 0$,

$$-\int_{a}^{b} y(py')' \, dx + \int_{a}^{b} yqy \, dx - \int_{a}^{b} y\lambda ry \, dx = 0$$

$$\Leftrightarrow -\int_{a}^{b} y(py')' \, dx + \int_{a}^{b} qy^{2} \, dx - \lambda \int_{a}^{b} ry^{2} \, dx = 0$$

$$\Rightarrow -pyy' \Big|_{a}^{b} + \int_{a}^{b} p(y')^{2} \, dx + \int_{a}^{b} qy^{2} \, dx - \lambda \int_{a}^{b} ry^{2} \, dx = 0$$

$$\Rightarrow \lambda = \left[\int_{a}^{b} p(y')^{2} \, dx + \int_{a}^{b} qy^{2} \, dx - pyy' \Big|_{a}^{b}\right] / \int_{a}^{b} ry^{2} \, dx \ge 0$$

As a side note, the **Rayleigh quotient**, $R[y] = \langle y, Ly \rangle / \langle y, ry \rangle$, is used extensively in analysis.

Note: Most authors modify the third condition above to instead require that the BCs satisfy $\alpha_1^2 + \alpha_2^2 > 0$ and $\alpha_3^2 + \alpha_4^2 > 0$ to define a regular SL problem. However, it is then less trivial (and not always true) that one can bound the eigenvalues below by 0 as in the above statement (though they can still be shown to be bounded and ordered in an increasing chain as above). One needs the first two

Oscillation theorem [Simplest version]: The k^{th} eigenfunction will have k zeroes on a < x < b ($k = 0, 1, 2, \cdots$).

Monotonicity theorem: Comparing two SL problems, SL and \widetilde{SL} , with the same boundary conditions, the eigenvalues will satisfy $\tilde{\lambda}_k > \lambda_k$ if

$$\tilde{p}(x) \ge p(x)$$
 and $\tilde{q}(x) \ge q(x)$ and $\tilde{r}(x) \le r(x)$ and $(\tilde{a}, b) \subseteq (a, b)$

and the strict inequality (or strict inclusion) holds in at least one of these cases.

2.9 Application: Linear Instability Analysis (Non-examinable)

As an application of the theory developed above, we can again consider the reaction-diffusion equation (9) in a specific context. Consider the system to model the density u(x,t) of some species which can survive in the interval $x \in (0, L)$ but for which the environment outside of this interval is hostile, and so the animals cannot live there. Within the domain, the species move via Fickian diffusion, and grow logistically (i.e., Fisher's Equation). This is essentially a model of Spruce budworm invasion, but we will not go into the biological context too much. Then a model for this species' density reads,

$$u_t = Du_{xx} + u\left(1 - \frac{u}{K}\right),\tag{34}$$

where D is the diffusion coefficient, and K the carrying capacity. We model the hostile environment with the Dirichlet boundary conditions u(0,t) = u(L,t) = 0. We assume an initial profile of the species given as $u(x,0) = u_0(x) \ge 0$, and want to know if this species will be able to survive or not in this region of space, and how this might depend on the parameters D, K, and L.

It is not possible to solve (34) analytically, but we can guess steady state solutions based on the form of the function f = u(1 - u/K). We note that the homogeneous solution u = K does not satisfy the Dirichlet conditions, and so is not suitable. The solution u = 0 on the other hand does, and nicely represents extinction. As the right hand side of (34) is identically 0 for this solution, once the population has become extinct it will remain so indefinitely. We then use a linear stability analysis to determine if a small initial density will grow away from this extinction state, or collapse onto it.

We consider a small perturbation ansatz of the form $u = 0 + \epsilon v(x, t)$, where $\epsilon \ll 1$ indicates the size of the perturbation. Substituting this into (2.9) and dividing the equation by ϵ we find,

$$v_t = Dv_{xx} + v\left(1 - \epsilon \frac{v}{K}\right) = Dv_{xx} + v + O(\epsilon).$$
(35)

Henceforth, we neglect terms of order ϵ , as is usual in linear stability analysis. Noting that (35) is a linear equation, we can perform separation of

variables and write v(x,t) = X(x)T(t), finding equations for the temporal and spatial parts. In particular, the spatial function X(x) will solve a linear boundary value problem for which we can find an infinite set of solutions explicitly, and the temporal part T(t) will be slaved to the spatial eigenvalues of the spatial BVP. You should find the solution of (35) now, and compare your solution to the 'quick and dirty' method shown below.

Knowing the form of the spatial operator, we can use the eigenfunctions associated with $Ly = y_{xx}$, together with the Dirichlet boundary conditions. These will be of the form $y_k = \sin(k\pi/L)$, for k = 1, 2, ..., in order to match the Dirichlet conditions. The time-dependent solution will be of the form $T(t) = \exp(\alpha t)$, where α will depend on the rest of the problem. We therefore consider the solution ansatz,

$$v(x,t) = \sum_{k=1}^{\infty} e^{\alpha_k t} \sin\left(\frac{xk\pi}{L}\right).$$
(36)

We note that if all of the (unknown) factors α_k are negative, then v(x,t) will decay over time and eventually return to the homogeneous steady state of 0. If, on the other hand, $\alpha_k > 0$ for some k, then this small population will grow as long as the initial distribution has some nonzero component of this eigenfunction. We now determine how to find these growth rates α_k .

Substituting (36) into (35).

$$\sum_{k=1}^{\infty} \alpha_k e^{\alpha_k t} \sin\left(\frac{xk\pi}{L}\right) = -D \sum_{k=1}^{\infty} \frac{k^2 \pi^2}{L^2} e^{\alpha_k t} \sin\left(\frac{xk\pi}{L}\right) + \sum_{k=1}^{\infty} e^{\alpha_k t} \sin\left(\frac{xk\pi}{L}\right).$$
(37)

We can then consider this term by term, for instance by multiplying by $\sin(\frac{xk\pi}{L})$ for a specific k and integrating across the domain. Doing this, and dividing out the functions, we find the infinite sequence of algebraic relations,

$$\alpha_k = -D\frac{k^2\pi^2}{L^2} + 1. \tag{38}$$

We immediately have that $\alpha_k < \alpha_j$ for k > j, so that the largest growth rate is α_1 . We then have that $\alpha_1 > 0$ if $D\pi^2 < L^2$, and hence have determined a condition in which a population will not become extinct which is a function of the model parameters. One interesting observation is that whether or not the species becomes extinct does not depend on K, although any actual stable species distribution (which we cannot compute using these methods) will depend on this parameter. See the course notes for B5.5 for further information and examples similar to this one.

Finally we remark that all of this can be generalized beyond the case of diffusion using the Sturm-Louiville theory developed above. One major application of these ideas about eigenfunction is precisely to be able to compute linear stability of more complicated models, even when analytically solving such nonlinear models is not feasible (which is true of almost all nonlinear problems).

3 Green's function

In this section we will develop an alternative approach to viewing and solving linear BVPs, using the *Green's function*.

3.1 Form of the eigenfunction expansion solution

Consider the form of the final solution obtained through the eigenfunction expansion approach. Taking Equation (17) one step further, we have

$$y(x) = \sum_{k=1}^{\infty} \frac{\langle f, w_k \rangle}{\lambda_k \langle y_k, w_k \rangle} y_k(x)$$

Aside: this requires all $\lambda_k \neq 0$. The case of zero eigenvalue has two subcases:

- $< f, w_k > \neq 0$: in this case, the BVP has no solution.
- $\langle f, w_k \rangle = 0$: in this case, the solution is not unique as any multiple of y_k (the eigenfunction that belongs to the zero eigenvalue) can be added to the solution.

This observation is directly linked to the Fredholm Alternative, which will be discussed in "Further Mathematical Methods" in HT.) Let $n_k = \langle y_k, w_k \rangle$ (normalisation), then:

$$y(x) = \sum_{k=1}^{\infty} \frac{1}{\lambda_k n_k} \left(\int_a^b f(t) w_k(t) dt \right) y_k(x)$$
$$= \int_a^b \left(\sum_{k=1}^{\infty} \frac{1}{\lambda_k n_k} w_k(t) y_k(x) \right) f(t) dt$$
$$= \int_a^b g(x,t) f(t) dt$$

where

$$g(x,t) = \sum_{k=1}^{\infty} \frac{w_k(t)y_k(x)}{\lambda_k n_k}.$$
(39)

Thus, we have constructed a solution to Ly = f in the form

$$y(x) = \int_{a}^{b} g(x,t)f(t) \, dt.$$
(40)

The function g(x,t) is called the Green's function (GF), and the form (39) is an eigenfunction expansion of g(x,t).

Of course, if we knew the Green's function, we would have the solution without any need for the expansion (i.e. no need for the eigenfunctions). The goal in this section is to understand the properties of the GF and how to construct it.

Side note: Observe that if $L = L^*$, then $w_k = y_k$ and:

$$g(x,t) = \sum \frac{1}{\lambda_k n_k} y_k(t) y_k(x)$$

In this case g(x,t) = g(t,x), and we have the important connection between a self-adjoint operator and a symmetric Green's function.

3.2 Inverse of differential operator

A nice way to think of the Green's function is in terms of inverting the differential operator. Think about the familiar equation $\mathbf{A}\vec{x} = \vec{b}$ from linear algebra, to be solved for the unknown vector \vec{x} . The solution is given by

$$\vec{x} = \mathbf{A}^{-1}\vec{b},$$

i.e. we find the solution by multiplying the inverse of the linear operator (matrix) by the inhomogeneous term. Once you know the inverse operator, you can solve the problem for any given vector \vec{b} . In the context of BVP's, L is a differential operator, so it stands to reason that the inverse operator involve integration, hence the form (40). Constructing the Green's function is analogous to finding the inverse of the matrix, once we have g we can write down the solution (40) for any forcing function f(x).

3.2.1 An example

There are numerous ways to construct a Green's function. We've already seen one: the eigenfunction expansion. Another way that you've probably seen before is via variation of parameters². This approach gives the Green's function in a piecewise form.

Let's look at a simple example. Consider the BVP:

$$Ly \equiv -y'' = f(x), 0 < x < 1$$

y(0) = y(1) = 0 (41)

The GF, via variation of parameters, is given by

$$g(x,\xi) = \begin{cases} \frac{-y_l(x)y_r(\xi)}{W(\xi)} & 0 < x < \xi\\ \frac{-y_l(\xi)y_r(x)}{W(\xi)} & \xi < x < 1 \end{cases} = \begin{cases} (1-\xi)x & 0 < x < \xi\\ (1-x)\xi & \xi < x < 1, \end{cases}$$
(42)

where $Ly_l = 0 = Ly_r$, $B_l(y_l) = 0$, $B_r(y_r) = 0$, and $W = y_l y'_r - y'_l y_r$ is the Wronskian.

The following properties are easily checked:

- The GF satisfies Lg = 0 if $x \neq \xi^3$
- $g(x,\xi)$ satisfies the boundary conditions as a function of x.
- g is continuous on the whole interval [0, 1]

 $^{^{2}}$ You will not be tested on this method, but if you would like to review the approach you might check out the textbook *Elementary Differential Equations and Boundary Value Problems*, by Boyce and DiPrima.

³Here by L we mean the operator acting on the x variable, i.e. derivatives are with respect to x – this is sometimes written $L_x g(x, \xi)$ to clarify.

• g is differentiable everywhere except at $x = \xi$, where it suffers a jump in the derivative.

These properties are, in fact, always true of the GF of a second order linear operator.⁴ To make sense of this, and to build some physical intuition, we shall need the notion of the delta function.

3.3 Green's function via delta function

To fix the context, consider stationary heat conduction in a rod:

$$-y''(x) = f(x) \qquad 0 < x < 1 \tag{43}$$

$$y(0) = 0, \ y(1) = 0.$$
 (44)

where y(x) is the temperature field and f(x) is a given heat source density.

3.3.1 Delta function

The function f(x) describes any heat added to, or removed from, the system by the outside world. As a simple scenario, consider a *point heat source*, say located at the middle of the rod. Physically, this would correspond to applying heat at a single point only. How would we describe such a situation mathematically? What should we use for the function f(x)?

The notion of a point source is described by the "delta function" δ , characterised by properties

$$\delta(x) = 0 \quad \forall x \neq 0, \qquad \int_{-\infty}^{\infty} \delta(x) \, dx = 1. \tag{45}$$

The first property captures the notion of a point function. The second property constrains the area under the curve (which you might think of as infinitely thin and infinitely high). This is an idealized point source at x = 0; a point source at x = a would be given by $\delta(x - a)$.

The problem is that no classical function satisfies (45) (think: any function that is non-zero only at a point is either not integrable or integrates to zero).

⁴Note, however, that the function y(x) satisfying Ly = f is continuously differentiable assuming continuously differentiable f, meaning that the integration with f(x) smooths out the discontinuity in g.

3.3.2 Approximating the delta function

One way around this is to replace δ by an approximating sequence of increasingly narrower functions with normalized area, i.e. $f_n(x)$ where



Figure 2: Hat functions, see equation (46).

Example: "hat" functions

$$f_n(x) = \begin{cases} 0 & \text{for } |x| > 1/n \\ n/2 & \text{for } |x| \le 1/n \end{cases}$$
(46)

You can verify the $f_n(x)$ approach $\delta(x)$ as $n \to \infty$.

3.3.3 Properties of delta function

We have defined δ by (45). We can use the approximating functions to obtain further properties.

Sifting property. What happens when δ is integrated against another function?

Let f(x) be a continuous function, and $F(x) = \int^x f(s) ds$ its antiderivative. Now consider approximating sequences:

$$\int_{-\infty}^{\infty} \delta(x-a) f(x) dx = \lim_{n \to \infty} \int_{-\infty}^{\infty} f_n(x-a) f(x) dx,$$

and if f_n are the hat functions (46),

$$= \lim_{n \to \infty} \int_{a-1/n}^{a+1/n} \frac{n}{2} f(x) dx = \lim_{n \to \infty} \frac{F(a+(1/n)) - F(a-(1/n))}{2/n}$$
$$= \lim_{s \to 0} \frac{F(a+s) - F(a-s)}{2s} = F'(a) = f(a).$$

Thus, we have

$$\int_{-\infty}^{\infty} \delta(x-a) f(x) dx = f(a) \quad \text{if } f \text{ is continuous at } a.$$
(47)

In particular,

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0) \quad \text{if } f \text{ is continuous at } x = 0.$$
(48)

Thus, the delta function can be seen to sift out the value of a function at a particular point.

Antiderivative of $\delta(x)$. The antiderivative of the delta function is the so-called Heaviside function,

$$\int_{-\infty}^{x} \delta(s) \mathrm{d}s = H(x) \equiv \begin{cases} 0 & x < 0\\ 1 & x > 0. \end{cases}$$
(49)

Note that (49) follows by integrating the sequence of approximating functions and showing that the limit is the Heaviside function. That is, if $H_n(x) = \int_{-\infty}^x f_n(s) ds$, then $\lim_{n\to\infty} H_n(x) = H(x)$. (We leave this detail as an exercise!)

3.3.4 Point heat source

Let's return to the heat conduction BVP with a point heat source of unit strength at the centre of the rod:

$$-y''(x) = \delta(x - 1/2), \quad 0 < x < 1$$
(50)

$$y(0) = y(1) = 0. (51)$$

Since $\delta(x - 1/2) = 0 \quad \forall x \neq 1/2$, this implies

$$-y''(x) = 0, \quad 0 < x < 1/2, \ 1/2 < x < 1.$$
(52)

We can easily solve (52) in each of the two separate domains [0, 1/2) and (1/2, 1] and then apply the BC (51). But be careful: there are two constants of integration for each domain, meaning *four* unknown constants total, and only *two* boundary conditions.

As you might expect (since $\delta(x - 1/2)$ has vanished from (52)), the extra two conditions come in at x = 1/2. To derive the extra conditions, imagine integrating equation (50) across x = 1/2:

$$\int_{1/2-}^{1/2+} -y''(x) \, dx = \int_{1/2-}^{1/2+} \delta(x-1/2) \, dx, \tag{53}$$

where 1/2-(1/2+) signifies just to the left (right) of 1/2. Using property (45) of the delta function, we have

$$-y']_{1/2-}^{1/2+} = 1 \quad \Rightarrow \quad y'(1/2+) - y'(1/2-) = -1.$$
 (54)

That is, the presence of the delta function defines a jump condition on y'.⁵

The other extra condition comes as a requirement that y(x) is continuous across the point source, that is

$$y]_{1/2-}^{1/2+} = 0. (55)$$

More on this condition below. Solving Equations (52), (51) together with extra conditions (54) and (55), we obtain the solution

$$y(x) = \begin{cases} \frac{x}{2} & 0 < x < 1/2\\ -\frac{x}{2} + \frac{1}{2} & 1/2 < x < 1. \end{cases}$$
(56)

3.3.5 Green's function construction

To motivate the construction of the Green's function, consider the heat conduction problem with an arbitrary heat source:

$$-y''(x) = f(x), \quad 0 < x < 1$$
(57)

$$y(0) = y(1) = 0. (58)$$

⁵Here, $y(\xi-) = \lim_{x\uparrow\xi} y(x)$, and $y(\xi+) = \lim_{x\downarrow\xi} y(x)$

Imagine now describing f by a distribution of point heat sources with varying strength; that is at point $x = \xi$ we imagine placing the point source $f(\xi)\delta(x-\xi)$.

The idea of the Green's function is to introduce such an extra parameter ξ , and consider the system

$$-g''(x,\xi) = \delta(x-\xi), \quad 0 < x < 1$$
(59)

$$g(0,\xi) = g(1,\xi) = 0.$$
(60)

Note that prime denotes differentiation with respect to x, while ξ is more like a place-holding variable. So, we have replaced f(x) by a delta function, in order to solve for the Green's function $g(x,\xi)$.

We have seen how to solve (59), (60) in the last section. The Green's function is

$$g(x,\xi) = \begin{cases} (1-\xi)x & 0 < x < \xi\\ (1-x)\xi & \xi < x < 1. \end{cases}$$
(61)

Notice that this is exactly the solution (42) one would obtain via variation of parameters.

How do we get back to the solution of Equations (57), (58)? For each ξ , the Green's function gives the solution if a point heat source of unit strength were placed at $x = \xi$. Conceptually, then, to get the full solution we must "add up" the point sources, scaled by the value of the heat source at each point:

$$y(x) = \int_0^1 g(x,\xi) f(\xi) \, d\xi.$$
 (62)

To verify that this is indeed a solution, we can substitute (62) into (57):

$$-y''(x) = \int_0^1 -g''(x,\xi)f(\xi) \, dx = \int_0^1 \delta(x-\xi)f(\xi) \, dx = f(x) \checkmark$$
(63)

3.4 General linear BVP

We now consider a general nth order linear BVP with arbitrary continuous forcing function,

$$Ly(x) = a_n y^{(n)}(x) + a_{n-1} y^{(n-1)}(x) + \dots + a_1 y'(x) + a_0 y(x) = f(x) \quad (64)$$

for a < x < b, where each $a_i = a_i(x)$ is a continuous function, and moreover $a_n(x) \neq 0 \forall x^6$. Along with Equation (64), we impose *n* boundary conditions, each a linear combination of *y* and derivatives up to $y^{(n-1)}$, evaluated at x = a, b. For instance, in the case n = 2, the general form is:

$$B_{1}y \equiv \alpha_{11}y(a) + \alpha_{12}y'(a) + \beta_{11}y(b) + \beta_{12}y'(b) = \gamma_{1}$$

$$B_{2}y \equiv \alpha_{21}y(a) + \alpha_{22}y'(a) + \beta_{21}y(b) + \beta_{22}y'(b) = \gamma_{2}.$$
(65)

3.5 General Green's Function

In the same way as in Section 3.3.4, to solve (64) with homogeneous BC

$$B_i y = 0, \quad i = 1 \dots n - 1.$$

we first determine the Green's function by solving

$$Lg(x,\xi) = \delta(x-\xi), \quad a < x < b$$

$$B_ig = 0.$$
(66)

As before,

$$Lg(x,\xi) = \delta(x-\xi)$$

implies

$$Lg(x,\xi) = 0$$
 on $a < x < \xi, \ \xi < x < b,$

i.e. we have a homogeneous problem to solve on two separate domains. As before, we require extra conditions, which come by integrating $Lg(x,\xi) = \delta(x-\xi)$ across $x = \xi$:

$$\int_{\xi^{-}}^{\xi^{+}} a_n g^{(n)}(x,\xi) + \dots + a_0 g(x,\xi) \ d\xi = \int_{\xi^{-}}^{\xi^{+}} \delta(x-\xi) \ dx.$$
(67)

The right hand side clearly integrates to one. If we were to perform an integration by parts on the first term of the left hand side, we would obtain

$$a_n(x)g^{(n-1)}(x,\xi)]_{\xi-}^{\xi+} + \int_{\xi-}^{\xi^+} (a_{n-1} - a'_n)g^{(n-1)} + \dots + a_0g(x,\xi) \ dx = 1.$$

This equation is balanced by setting a jump condition on the n-1st derivative:

$$g^{(n-1)}(x,\xi)]_{\xi-}^{\xi+} = 1/a_n(\xi),$$

⁶We will not cover the case where $a_n(x) = 0$ somewhere in the domain, as such a singular point can fundamentally change the solution structure, as the problem becomes singular there – see the notes for C5.5 for further information.

and taking all lower derivatives to be continuous across $x = \xi$:

$$g^{(j)}(x,\xi)]_{\xi-}^{\xi+} = 0, \quad j = 0, 1, \dots n-2.$$

Once the Green's function is determined, the solution to the BVP is given by

$$y(x) = \int_{a}^{b} g(x,\xi) f(\xi) \, d\xi.$$
 (68)

3.5.1 Example: Biharmonic Equation

Let's look at an example of a Green's function for a fourth-order operator to see how the above ideas generalize, though be warned that the algebra can become very tedious. Consider the problem,

$$Lu = \frac{d^4u}{dx^4} - u = f(x), \quad u(0) = 0, \quad u(1) = 0, \quad u''(0) = 0, \quad u''(1) = 0.$$
(69)

As noted before, there are several different ways to find the Green's function, but it will always satisfy the same equation. Namely,

$$Lg(x,\xi) = \frac{d^4g}{dx^4} - g = \delta(x-\xi), \ g(0,\xi) = 0, \ g(1,\xi) = 0, \ g''(0,\xi) = 0, \ g''(1,\xi) = 0$$
(70)

As before, we can look for the general solutions of Lu = 0 to obtain functions of x which must constitute the full set of solutions, and then choose constants to match both the boundary conditions and the conditions at $x = \xi$. This homogeneous equation admits general solutions of the form $u = A \sinh(x) + B \cosh(x) + C \sin(x) + D \cos(x)$, where these four coefficients will be different on each side of $x = \xi$, and may depend on ξ (but not on x). Here I've chosen to use $\sinh(x)$ and $\cosh(x)$, but these are equivalent to working with e^x and e^{-x} , though again the algebraic details can be easier in one form or another.

In general this will lead to a system of 8 unknowns and 8 constraints, which is quite hard to deal with. As an alternative, we can pick two sets of solutions which satisfy the boundary conditions ahead of time, and as long as the resulting set of solutions can span the space of homogeneous solutions given above by y, then we can worry only about the matching conditions at $x = \xi$. We can therefore choose $u_{\ell} = A \sinh(x) + B \sin(x)$, and $u_r = C \sinh(1-x) + D \sin(1-x)$. Then it is easy to see that $u_{\ell}(0) = u''_{\ell}(0) = 0$, and $u_r(1) = u''_r(1) = 0$. We then let the coefficients A, B, C, D depend on ξ , and consider the point $x = \xi$. We have the four conditions $u_{\ell} = u_r$, $u'_{\ell} = u'_r$, $u''_{\ell} = u''_r$, and $u'''_r - u'''_{\ell} = 1$. Once these coefficients are found (which is often a substantial amount of work, unless there's a trick), the Green's function can be written as,

$$g(x,\xi) = \begin{cases} A(\xi)\sinh(x) + B(\xi)\sin(x) & 0 < x < \xi, \\ C(\xi)\sinh(1-x) + D(\xi)\sin(1-x) & \xi < x < 1, \end{cases}$$

and the general solution of (69) as,

$$y = \int_0^1 g(x,\xi) f(\xi) d\xi.$$

3.6 Another view

There is one more way of viewing the GF. Start from Ly(x) = f(x), and take an inner product with $G(x,\xi)$ on both sides of the equation⁷. We are not assuming we know G, rather we want to find properties it should satisfy for us to solve the equation. We obtain

$$\langle Ly, G \rangle = \langle G(x,\xi), f(x) \rangle = \int_{a}^{b} G(x,\xi) f(x) \, dx.$$
 (71)

(Note the integration is over x). Now, using the adjoint, we can write

$$\langle Ly, G \rangle = \langle y, L^*G \rangle \tag{72}$$

The idea now is to isolate y. This can be accomplished if

$$L^*G(x,\xi) = \delta(x-\xi) \tag{73}$$

in which case the right hand side leaves just $y(\xi)$, and we have the solution

$$y(\xi) = \int_{a}^{b} G(x,\xi)f(x) \, dx.$$
 (74)

Comparing with our previous construction, here the big difference is that the GF is constructed through the adjoint operator – hence we will refer to

 $^{{}^{7}}G$ will be the Green's function, but not quite the same one we've constructed, so I am differentiating by using capital G.

this as the adjoint Green's function. Compare the form of solution with the form (40):

$$y(x) = \int_{a}^{b} g(x,t)f(t) \, dt,$$
(75)

we see the subtle difference that in (74) we integrate over the first variable of the adjoint GF, and the second variable of the GF. For a self-adjoint operator, the constructions are the same and we must get the same GF, and indeed as we've stated, the GF for a self-adjoint operator is symmetric.

4 Distributions

In Section 3 we say how the Green's function can be a valuable tool in solving BVPs. However, constructing the GF required us to define the "delta function", which is not really a functionat all, and at best a limit of functions. We also saw that the GF suffers a discontinuity in the n - 1st derivative. We now take a short detour to consider these issues in more detail, by introducing the theory of distributions.

Perhaps the most important feature of the δ -"function": when integrated against a continuous function, it sifts out the value at x = 0:

$$\int_{-\infty}^{\infty} \delta(x) f(x) \mathrm{d}x = f(0).$$

It is the operation of δ on another function that defines the property. This is the key idea in the theory of distributions, in which a generalized function is only thought of in relation to how it affects other functions when "integrated" against them.

We define the delta <u>distribution</u> δ such that when it operates on a <u>test function</u> ϕ , it "sifts out" the value $\phi(0) \in \mathbb{R}$. We write this as

$$\langle \delta, \phi \rangle \equiv \phi(0),$$

where δ is the δ -distribution and ϕ is the test function. $\langle \delta, \phi \rangle$ reads as " δ applied to ϕ ".

We will generalise this idea momentarily. First, we need some tools and terminology.

<u>Test functions</u> $\phi : \mathbb{R} \to \mathbb{R}$ $\phi \in C_0^{\infty}(\mathbb{R})$, which is short for:

- $\phi \in C^{\infty}(\mathbb{R})$ differentiable any number of times
- ϕ has "compact support", i.e. supp $\phi \subseteq [-X, X]$ for some X > 0, i.e. $\phi(x) = 0 \quad \forall x \notin [-X, X].$

So a test function is infinitely smooth, has no kinks or corners, and vanishes outside a finite region.



Figure 3: Sample test function, corresponding to (76)

One can show (for all integer $n \ge 0$):

$$\lim_{x\uparrow a+\epsilon} \frac{d}{dx^n} \phi_{C;\epsilon}(x) = 0$$
$$\lim_{x\downarrow a-\epsilon} \frac{d}{dx^n} \phi_{C;\epsilon}(x) = 0$$

4.1 Weak derivative

Having defined test functions, we can generalise the notion of a derivative. Start with the classical definition: let u(x) be a continuously differentiable function with derivative f(x), so u'(x) = f(x). Now, multiply each side of the equation by a test function ϕ and integrate over \mathbb{R} :

$$\int_{\mathbb{R}} u'\phi \, dx = \int_{\mathbb{R}} f\phi \, dx. \tag{77}$$

Integrating the LHS by parts and using the compact support of ϕ , we obtain

$$-\int_{\mathbb{R}} u\phi' \, dx = \int_{\mathbb{R}} f\phi \, dx. \tag{78}$$

The idea of the weak derivative is to think of (78) as the *definition* of a derivative. That is, we say f is the *weak derivative* of u if (78) holds for all test functions $\phi \in C_0^{\infty}(\mathbb{R})^8$. The value is that this definition does not require u to be differentiable, just integrable. Of course, if u is continuously differentiable, the weak derivative and the ordinary one will agree, but a function that is not continuously differentiable can still have a weak derivative, where essentially the integration smooths out discontinuities.

4.2 Distribution definition

This leads us to the notion of a distribution, or a generalised function. A distribution is not defined at points, but rather it is a global object defined in terms of its action on test functions. To be more precise:

Definition: A distribution u is a functional mapping test functions $\phi \in C_0^{\infty}(\mathbb{R})$ to real numbers,

$$u: \phi \in C_0^{\infty}(\mathbb{R}) \mapsto \langle u, \phi \rangle \in \mathbb{R} \qquad (\langle u, \phi \rangle \text{ instead of } u(\phi)) \tag{79}$$

where the mapping is *linear* and *continuous*. While we have motivated the action $\langle u, \phi \rangle$ as meaning integration, this is not a requirement.

Linearity is straightforward, and means

$$\langle u, \alpha \phi + \beta \psi \rangle = \alpha \langle u, \phi \rangle + \beta \langle u, \psi \rangle \qquad \forall \alpha, \beta \in \mathbb{R} \quad \forall \phi, \psi \in C_0^{\infty}(\mathbb{R})$$
(80)

⁸We can also confine to smaller intervals, for instance $\phi \in C_0^{\infty}(a, b)$ means the test functions have compact support in a bounded subset of (a, b).

Continuity is slightly more technical; it means that if ϕ_n is a sequence of test functions that converges to zero,

$$\phi_n(x) \to 0$$
 as $n \to \infty$

then

$$\langle u, \phi_n \rangle \to 0$$
 (81)

as a sequence of real numbers.

To show continuity, we need to be able to switch the order of "the action of the distribution" (integration) and the limit, that is (81) will hold if

$$\lim_{n \to \infty} \langle u, \phi_n \rangle = \langle u, \lim_{n \to \infty} \phi_n \rangle.$$

It turns out that we can do this if the following holds:

(*) $\forall X > 0$ there exists C > 0, and integer $N \ge 0$, such that

$$|\langle u, \phi \rangle| \le C \sum_{m \le N} \max_{-\infty \le x \le \infty} \left| \frac{\mathrm{d}^m \phi}{\mathrm{d}x^m} \right|$$

 $\forall \phi \text{ with support in } [-X, X].$

For our purposes we will want to show (*) to show continuity, and in fact you can take this as the definition of continuity.

Examples

Delta distribution

$$\langle \delta, \phi \rangle = \phi(0)$$

linearity: \checkmark

continuity, check (*): $|\langle \delta, \phi \rangle| = |\phi(0)| \leq \max_{-X < x < X} |\phi(x)| \quad \forall \phi \text{ with support of } \phi \text{ in } [-X, X].$ i.e. condition (*) is satisfied with C = 1, N = 0.

Generalisation

Let $a \in \mathbb{R}$, $n \ge 0$. Define $\langle D_n, \phi \rangle = \phi^{(n)}(a)$ (*n*th derivative). This is a distribution (to be proved in a problem sheet). **Functions as distributions.** For any locally integrable function f(x), a natural distribution is defined by

$$\langle f, \phi \rangle = \int_{-\infty}^{\infty} f(x)\phi(x) \mathrm{d}x$$

Check:

Well-defined, $\langle f, \phi \rangle \in \mathbb{R} \ \forall \phi \in C_0^{\infty}(\mathbb{R})$ and linear.

Continuity? (*): Let X > 0 be given. Claim (*) holds for

$$C = C(X) = \int_{-X}^{X} |f(x)| dx \text{ and } N = 0:$$
$$|\langle f, \phi \rangle| = |\int_{-\infty}^{\infty} f(x)\phi(x) dx| = |\int_{-X}^{X} f(x)\phi(x) dx|$$

which by the estimation lemma

$$\leq \int_{-X}^{X} |f(x)| \mathrm{d}x \max_{-X < x < X} (|\phi(x)|) = C \max_{-\infty < x < \infty} (|\phi(x)|)$$

Remark: Different continuous functions induce different distributions.

Heaviside function H(x)

$$\langle H, \phi \rangle = \int_{-\infty}^{\infty} H(x)\phi(x) dx = \int_{0}^{\infty} \phi(x) dx$$

Can check linearity, continuity as an exercise.

<u>Remark</u>: Different functions can lead to the same distribution. Distributions induced by *integrable* functions are called *regular* distributions; singular distributions if not. The δ -distribution is an example of a singular distribution.

4.3 Operations on distributions

Now we consider some operations that can be performed on distributions. Let u_1, u_2, u be *distributions*, and f_1, f_2, f be integrable *functions* (or the regular distributions induced by them). The notion of integration is not required for distributions, but the rules for distributions are consistent with those for locally integrable functions.

Linear combinations of distributions. Let $\alpha_1, \alpha_2 \in \mathbb{R}$.

$$\begin{aligned} \langle \alpha_1 f_1 + \alpha_2 f_2, \phi \rangle &= \int_{-\infty}^{\infty} (\alpha_1 f_1(x) + \alpha f_2(x)) \phi(x) \mathrm{d}x \\ &= \alpha_1 \int_{-\infty}^{\infty} f_1(x) \phi(x) \mathrm{d}x + \alpha_2 \int_{-\infty}^{\infty} f_2(x) \phi(x) \mathrm{d}x \\ &= \alpha_1 \langle f_1, \phi \rangle + \alpha_2 \langle f_2, \phi \rangle \end{aligned}$$

Thus, <u>define</u> $\alpha_1 u_1 + \alpha_2 u_2$ for general distributions u_1, u_2 via

$$\langle \alpha_1 u_1 + \alpha_2 u_2, \phi \rangle \equiv \alpha_1 \langle u_1, \phi \rangle + \alpha_2 \langle u_2, \phi \rangle \quad \forall \phi \in C_0^\infty(\mathbb{R})$$

If u_1, u_2 are distributions, is $\alpha_1 u_1 + \alpha_2 u_2$ a distribution? We need to check linearity and continuity, but we'll skip this here.

Differentiation of distributions. Differentiation follows the weak derivative formulated earlier. That is, for a general distribution u, <u>define</u>

$$\langle u', \phi \rangle \equiv -\langle u, \phi' \rangle \qquad \forall \phi \in C_0^\infty(\mathbb{R})$$

If u is distribution, can we be sure that $u': \phi \mapsto -\langle u, \phi' \rangle$ is also a distribution? (It is! – try it as an exercise.)

Example. Let H be the Heaviside function, or the distribution it induces, i.e.

$$\langle \underbrace{H}_{H\text{-distribution}}, \phi \rangle \equiv \int_{-\infty}^{\infty} \underbrace{H(x)}_{H\text{-function}} \phi(x) \mathrm{d}x = \int_{0}^{\infty} \phi(x) \mathrm{d}x$$

Show that $H' = \delta$.

Translation: similar considerations as before, upshot $(a \in \mathbb{R}, u \text{ distr})$:

$$\langle u(x-a), \phi(x) \rangle \stackrel{\text{chg of var}}{=} \langle u(y), \phi(y+a) \rangle = \langle u(x), \phi(x+a) \rangle$$

Example: $\langle \delta(x-a), \phi(x) \rangle = \langle \delta(x), \phi(x+a) \rangle = \phi(a)$

Multiplication: let a(x) be an infinitely differentiable function. We define

$$\langle au, \phi \rangle = \langle u, a\phi \rangle.$$

Convergence of a sequence of distributions u, u_1, u_2, \ldots distributions. Convergence $u_j \rightarrow u$ as $j \rightarrow \infty$ means:

$$\lim_{j \to \infty} \langle u_j, \phi \rangle = \langle u, \phi \rangle \qquad \forall \phi \in C_0^\infty(\mathbb{R})$$

Similarly: if $u(\alpha)$ is a family of distributions with a continuous parameter α , then

convergence $u(\alpha) \to u(\alpha_0)$ for $\alpha \to \alpha_0$ means:

$$\lim_{\alpha \to \alpha_0} \langle u(\alpha), \phi \rangle = \langle u(\alpha_0), \phi \rangle \qquad \forall \phi \in C_0^\infty(\mathbb{R})$$

4.4 Distributed solutions

Consider the equation

$$Lu \equiv a_2 u'' + a_1 u' + a_0 u = f.$$

We have always thought about the *classical solution*, that is a twice continuously differentiable function u(x) that satisfies the differential equation identically, i.e. we can take derivatives of u, substitute in, and the equation checks at every point. With distribution theory and the notion of a generalised function, we now can define a *distributed solution*. That is, if u and f are distributions, then Lu is a distribution, defined by the action

$$\langle Lu, \phi \rangle = \langle a_2 u'', \phi \rangle + \langle a_1 u', \phi \rangle + \langle a_0 u, \phi \rangle = \langle u, (a_2 \phi)'' \rangle - \langle u, (a_1 \phi)' \rangle + \langle u, a_0 \phi \rangle \stackrel{\text{define}}{=} \langle u, L^* \phi \rangle.$$

$$(82)$$

Here L^* is the formal adjoint operator. We say that u is a distributed solution to Lu = f if

$$\langle u, L^*\phi \rangle = \langle f, \phi \rangle$$

holds for all test functions ϕ . We highlight again that a function need not be differentiable in the ordinary sense to satisfy this definition; hence, distributions provide a way to have well-defined solutions that may have issues in the classical sense.

In particular, this construction of a distributed solution gives us a new way to interpret the Green's function. Since δ is really a distribution or a generalised function, the equation $Lg = \delta(x - \xi)$ should be interpreted in the distributional sense,

$$\langle Lg, \phi \rangle = \langle \delta(x - \xi), \phi \rangle$$

 $\langle q(x, \xi), L^* \phi \rangle = \phi(\xi).$

or

Moreover, since the Green's function that we construct is not twice continuously differentiable, it is really a distributed solution. Alternatively, if we interpret $Lg = \delta(x - \xi)$ as meaning that Lg = 0 everywhere that $x \neq \xi$, then using the properties of δ we can work purely in the "classical" sense. In fact, the final solution of Ly = f, obtained by integration with g, is continuous and a classical solution.

Final thoughts: If you are interested in distribution theory, it is at the core of functional analysis. Moreover, the idea of weak formulations has great use in finite element methods. For us, distribution theory is somewhat of a detour for this course. One could proceed to write things in a distributional sense anytime we encounter a 'delta function', but we can as well recognise delta as the limit of continuous functions and satisfying certain properties, thus in effect translating to a classical system. Unless we are specifically interested in a distributional aspect, the latter will be our approach.