.

1B METHODS LECTURE NOTES

Richard Jozsa, DAMTP Cambridge
rj310@cam.ac.uk
October 2013

PART I:

Fourier series, Self adjoint ODEs

PREFACE

These notes (in four parts) cover the essential content of the 1B Methods course as it will be presented in lectures. They are intended be self-contained but they should not be seen as a full substitute for other good textbooks, which will contain further explanations and more worked examples. I am grateful to the previous lecturer of this course, Dr Colm-Cille Caulfield, for making his notes available to me; they were very useful in forming a basis for the notes given here.

The term "mathematical methods" is often understood to imply a kind of *pragmatic* attitude to the mathematics involved, in which our principal aim is to develop actual explicit methods for solving real problems (mostly solving ODEs and PDEs in this course), rather than a carefully justified development of an associated mathematical theory. With this focus on applications, we will not give proofs of some of the theorems on which our techniques are based (being satisfied with just reasonably accurate statements). Indeed in some cases these proofs would involve a formidable foray into subjects such as functional analysis and operator theory. This "mathematical methods" attitude is sometimes frowned upon by pure-minded mathematicians but in its defence I would make two points: (i) developing an ability to apply the techniques effectively, provides a really excellent basis for later appreciating the subtleties of the pure mathematical proofs, whose considerable abstractions and complexities if taken by themselves, can sometimes obfuscate our understanding; (ii) much of our greatest mathematics arose in just this creatively playful way – of cavalierly applying not-yet-fully-rigorous techniques to obtain answers, and only later, guided by gained insights, developing an associated rigorous mathematical theory. Examples include manipulation of infinite series (without worrying too much about exact convergence criteria), use of infinitesimals in the early development of calculus, even the notion of a real number itself, the use of the Dirac delta function (allowing "infinity" as a value, but in a "controlled" fashion) and many more. Thus I hope you will approach and enjoy the content of this course in the spirit that is intended.

Richard Jozsa
October 2013

1 FOURIER SERIES

The subject of Fourier series is concerned with functions on $\mathbb{R}$ that are periodic, or equivalently, are defined on a bounded interval $[a, b)$ which may then be extended periodicallly to all of $\mathbb{R}$. A function f on $\mathbb{R}$ is **periodic with period** T if $f(t+T) = f(t)$ for all t (and conventionally we take the smallest such T). Thus f is fully specified if we give its values only on $[0, T)$ or any other interval of length at least T.

Basic example: $S(t) = A \sin wt$ and $C(t) = A \cos wt$.
A is the **amplitude**. Interpreting the variable t as time, we have:
period $T = 2\pi/w =$ time interval of a single wave,
frequency $f = w/2\pi = 1/T =$ number of waves per unit time,
angular frequency $f_{\text{ang}} = 2\pi/T = w =$ number of waves in a 2π interval (useful if viewing t as an angle in radians).
Sometimes the independent variable is space x e.g. $f(x) = A \sin kx$ and we have:
wavelength $\lambda = 2\pi/k =$ spatial extent of one wave,
wavenumber $1/\lambda = k/2\pi =$ number of waves in a unit length,
angular wavenumber $k = 2\pi/\lambda =$ number of waves in a 2π distance.
Beware: although w resp. k are *angular* frequency resp. wavenumber, they are often referred to simply as frequency resp. wavenumber, and the terminology should be clear from the context.

In contrast to the infinitely differentiable trig functions above, in applications we often encounter periodic functions that are not continuous (especially at $0, T, 2T, \ldots$) but which are made up of continuous pieces e.g. the sawtooth $f(x) = x$ for $0 \le x < 1$ with period 1; or the square wave $f(x) = 1$ for $0 \le x < 1$ and $f(x) = 0$ for $1 \le x < 2$ with period 2.

1.1 Orthogonality of functions

Recall that for vectors, say 2-dimensional real vectors

$$\underline{u} = a\underline{i} + b\underline{j} \qquad \underline{v} = c\underline{i} + d\underline{j}$$

we have the notion of orthonormal basis $\underline{i}, \underline{j}$ and inner product $\underline{u} \cdot \underline{v}$ which we'll write using a **bracket notation** $(\underline{u}, \underline{v}) = ac + bd$ (not to be confused with an open interval! - the meaning should always be clear from the context!). For complex vectors we use $(\underline{u}, \underline{v}) = a^*c + b^*d$ where the star denotes complex conjugation. $\underline{u}$ is normalised if $(\underline{u}, \underline{u}) = 1$ and $\underline{u}$ and $\underline{v}$ are orthogonal if $(\underline{u}, \underline{v}) = 0$.

Consider now the set of all (generally complex-valued) functions on an interval $[a, b]$. These are like vectors in the sense that we can add them (pointwise) and multiply them by scalars. Introduce the **inner product of two functions** $f, g : [a, b] \to \mathbb{C}$ as follows:

$$(f, g) = \int_a^b f^*(x) g(x) dx. \tag{1}$$

Note that this even *looks* rather like an 'infinite dimensional' version of the standard inner product formula, if we think of the function values as vector components parameterised by x i.e. we multiply corresponding values and "sum" (integrate) them up. (f,f) is called the **squared norm** of f and **two functions are orthogonal** if $(f,g)=0$. Note that $(f,g)=(g,f)^*$ so if either is zero then the other is too.

Sometimes we'll restrict the class of functions by imposing further boundary conditions (BCs) that are required to have the following property: if f and g satisfy the conditions then so does $c_1 f + c_2 g$ for any constants c_1, c_2. Such BCs are called **homogeneous BCs** and the resulting class of functions will always still form a vector space (i.e. be closed under linear combinations).

Example. For functions on $[0,1]$ the following BCs are homogeneous BCs: (a) $f(0)=0$, (b)$f(0)=f(1)$, (c) $f(0)+2f'(1)=0$. The following BCs are not homogeneous: (a) $f(0)=3$, (b) $f(0)+f'(1)=1$.

Important example of orthogonality: On the interval $[0,2L]$ consider

$$S_m(x)=\sin\frac{m\pi x}{L} \qquad C_n(x)=\cos\frac{n\pi x}{L} \qquad m,n=0,1,2,\ldots$$

Note that S_m (for $m\neq 0$) comprises m full sine waves in the interval $[0,2L]$ (and similarly for C_n). To calculate their inner products we can use the standard trig identities

$$\begin{aligned}
\cos A\cos B &= \frac{1}{2}[\cos(A-B)+\cos(A+B)]\\
\sin A\sin B &= \frac{1}{2}[\cos(A-B)-\cos(A+B)]\\
\sin A\cos B &= \frac{1}{2}[\sin(A+B)+\sin(A-B)].
\end{aligned}$$

We get for example, for $m,n\neq 0$

$$\begin{aligned}
(S_m,S_n) &= \int_0^{2L}\sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx\\
&= \frac{1}{2}\int_0^{2L}\cos\frac{(m-n)\pi x}{L}dx-\frac{1}{2}\int_0^{2L}\cos\frac{(m+n)\pi x}{L}dx\\
&= \begin{cases} 0 \text{ if } m\neq n.\\ L \text{ if } m=n.\end{cases}
\end{aligned}$$

More concisely, using the Kronecker delta

$$(S_m,S_n)=L\delta_{mn} \qquad m,n\neq 0 \tag{2}$$

so the rescaled set of functions $\frac{1}{\sqrt{L}}S_n(x)$ for $n=1,2,\ldots$ is an *orthonormal* set.

Similarly you can easily derive that for all $m,n=1,2,\ldots$ we have

$$\begin{gathered}(C_m,C_n)=L\delta_{mn}\\ (C_m,S_n)=(S_m,C_n)=0.\end{gathered} \tag{3}$$

Finally consider the cases with $m=0$ or $n=0$: S_0 is identically zero so we exclude it whereas $C_0(x)=1$ and it is easy to see

$$(C_0,C_0)=2L \qquad (C_0,C_m)=(C_0,S_m)=0 \quad \text{for all } m=1,2,\ldots$$

Putting all this together we see that the infinite set of functions $\mathcal{B} = \{\frac{1}{\sqrt{2}}C_0, S_1, C_1, S_2, C_2, \ldots\}$ is an orthogonal set with each function having norm $\sqrt{L}$. Indeed it may be shown (but not proved in this methods course...) that these functions constitute a **complete** orthogonal set, or an orthogonal basis for the space of all functions on $[0, 2L]$ (or functions on $\mathbb{R}$ with period $2L$) in the same sense that $\underline{i}, \underline{j}$ is a complete orthogonal set for 2-dimensional vectors – it is possible to represent any (suitably well behaved) function as a (generally infinite) series of functions from $\mathcal{B}$. Such a series is called a Fourier series.

1.2 Definition of a Fourier series

We can express any 'suitably well-behaved' (cf later for what this means) periodic function $f(x)$ with period $2L$ as a **Fourier series**:

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right)\right], \tag{4}$$

where a_n and b_n are constants known as the **Fourier coefficients** of f, (This expression applies also if f is a complex-valued function in which case the coefficients a_n and b_n are themselves complex numbers – we can just treat the real and imaginary parts of any such complex-valued f as separate real functions).

The Fourier series expansion will also apply to (suitably well behaved) *discontinuous* functions: if f is discontinuous at x then the LHS of eq. (4) is replaced by

$$\frac{f(x_+) + f(x_-)}{2}$$

where $f(x_+) = \lim_{\xi\downarrow x} f(\xi)$ and $f(x_-) = \lim_{\xi\uparrow x} f(\xi)$ are the right and left limits of f as we approach x from above and below respectively. Thus the Fourier series will converge to the *average value* of f across a jump discontinuity. Indeed in our present context this provides a convenient way to re-define the value of function at a bounded discontinuity e.g. we would replace the step function "$f(x) = 0$ if $x \leq 0$ and $f(x) = 1$ if $x > 0$" by the function "$g(x) = 0$ if $x < 0$, $g(0) = \frac{1}{2}$ and $g(x) = 1$ if $x > 0$". Often, this subtlety will be glossed over, and the left hand side will just be written as $f(x)$ (as in eq. (4)), with the behaviour at a bounded discontinuity being understood.

Determining the a_n and b_n is easy by exploiting the orthogonality of the sines and cosines. In terms of our previous notation of S_m and C_n we can write eq. (4) as

$$f(x) = a_0(\frac{1}{2}C_0) + \sum_{n=1}^{\infty} a_n C_n(x) + b_n S_n(x). \tag{5}$$

Consider now

$$(S_m, f) = \int_0^{2L} f(x) \sin\frac{m\pi x}{L} dx.$$

Substituting the RHS of eq. (5) and assuming it is okay to swap the order of summation and integration, we get

$$(S_m, f) = a_0(S_m, \frac{1}{2}C_0) + \sum_{n=1}^{\infty} a_n(S_m, C_n) + b_n(S_m, S_n).$$

According to the orthogonality relations eqs. (2,3) all inner products on RHS are zero except for (S_m, S_m) which is L. Hence we get $(S_m, f) = b_m L$ i.e.

$$b_m = \frac{1}{L}\int_0^{2L} f(x)\sin\frac{m\pi x}{L}dx \qquad m = 1, 2, \dots \tag{6}$$

Similarly by taking inner products of eq.(5) with C_m we get

$$a_m = \frac{1}{L}\int_0^{2L} f(x)\cos\frac{m\pi x}{L}dx \qquad m = 0, 1, 2, \dots \tag{7}$$

The factor of $\frac{1}{2}$ in the a_0 term of eq. (4) conveniently makes the a_m formula eq. (7) valid for m both zero and nonzero (recalling that $(C_0, C_0) = 2L$ but $(C_m, C_m) = L$ for $m \neq 0$).

Remarks

(i) The constant term $a_0/2$ equals the average value $\langle f \rangle = \frac{1}{2L}\int_0^{2L} f(x)\,dx$ of f over its period and then subsequent sine and cosine terms 'build up' the function by adding in terms of higher and higher frequency. Thus the Fourier series may be thought of as the decomposition of any signal (or function) into an infinite sum of waves with different but discrete wavelengths, with the Fourier coefficients defining the amplitude of each of these countably-many different waves.

(ii) The range of integration in the above formulas can be taken to be over any single period. Often it's more convenient to use the symmetrical range $\int_{-L}^{L}$.

(iii) Warning – if we start with a function having period T, be careful to replace L in the above formulas by $T/2$ (since above, we wrote the period as $2L$!)

Dirichlet conditions

So, what is meant by a 'well-behaved' function in the definition of a Fourier series? Here it is defined by the **Dirichlet conditions**: a periodic function $f(x)$ with period T is said to satisfy the Dirichlet conditions if f is bounded and has a finite number of maxima, minima and discontinuities on $[0, T)$ (and hence also $\int_0^T |f(x)|dx$ is well-defined). Then we have the theorem (not proved in this course):

Basic theorem: If f satisfies the Dirichlet conditions then f has a unique Fourier series as in eq. (4) with coefficients given by eqs. (7,6). This series converges to $f(x)$ at all points where f is continuous, and converges to the average of the left and right hand limits at all points where f is discontinuous.

Smoothness and order of Fourier coefficients

According to the Dirichlet conditions, it is possible to establish a Fourier series representation of a certain kind of discontinuous function. More generally it can be shown that the amount of non-smoothness is reflected by the rate at which the Fourier coefficients decay with n, as follows.

Theorem. Suppose that the p^{th} derivative of f is the lowest derivative that is discontinuous somewhere (including the endpoints of the interval). Then the Fourier coefficients for f fall off as $O[n^{-(p+1)}]$, as $n \to \infty$. Thus smoother functions (i.e. larger p) have coefficients falling off faster, and hence better convergence properties of the Fourier series.

Example
Consider the sawtooth function having period $2L$, given by:
$f(x) = x$ for $-L \leq x < L$, and repeating periodically outside $[-L, L)$.

Since the function is odd, we immediately get $a_n = 0$ for all n.
Integration by parts shows (as you can check), that

$$\begin{aligned} b_m &= \frac{2L}{m\pi}(-1)^{m+1}, \\ f(x) &= \frac{2L}{\pi}\left[\sin\left(\frac{\pi x}{L}\right) - \frac{1}{2}\sin\left(\frac{2\pi x}{L}\right) + \frac{1}{3}\sin\left(\frac{3\pi x}{L}\right) + \ldots\right]. \end{aligned} \tag{8}$$

This series is actually very slowly convergent – the smoothness parameter p above is zero in this example and indeed the coefficients fall off only as $O(1/n)$, as expected. In the figure we plot a few of its partial sums $f_N(x)$:

$$f_N(x) \equiv \sum_{n=1}^{N} b_n \sin\left(\frac{n\pi x}{L}\right).$$

Note that the series converges to 0 at $x = \pm L$ i.e. to the average value across these jump discontinuities.

The Gibbs phenomenon

Looking at the partial sums $f_N(x)$ for the discontinuous sawtooth function as plotted in figure 1, we can see that there is a persistent overshoot at the discontinuity $x = \pm L$. This is actually a general feature of Fourier series' convergence near any discontinuity and is called the Gibbs-Wilabraham phenomenon. It is illustrated even more clearly in figure 2, showing partial sums for the square wave function. These are pictorial illustrations and on example sheet 1 (question 5) you can work through a derivation of the Gibbs phenomenon. Although the sequence of partial sums f_N, $N = 1, 2, \ldots$ of the Fourier series of a function f (satisfying the Dirichlet conditions) always converges *pointwise* to f, the Gibbs phenomenon implies that the convergence is *not uniform* in a region around a discontinuity. [Recall that f_N converges to f pointwise if for each x and for each $\epsilon > 0$ there is an integer N_0 (which *can depend on* x as well as on ϵ) such that $|f_N(x) - f(x)| < \epsilon$ for all $N > N_0$. If for each $\epsilon > 0$, N_0 can be chosen to be independent of x, then the convergence is said to be uniform.]

Example/Exercise
The integral of the sawtooth function: $f(x) = x^2/2$, $-L \leq x \leq L$

As an exercise, show that the Fourier series representation of this function is

$$\frac{x^2}{2} = L^2\left[\frac{1}{6} + 2\sum_{n=1}^{\infty}\frac{(-1)^n}{(n\pi)^2}\cos\left(\frac{n\pi x}{L}\right)\right]. \tag{9}$$

Note that the coefficients fall off as $O(1/n^2)$, consistent with the fact that f is continuous but has discontinuous first derivative.

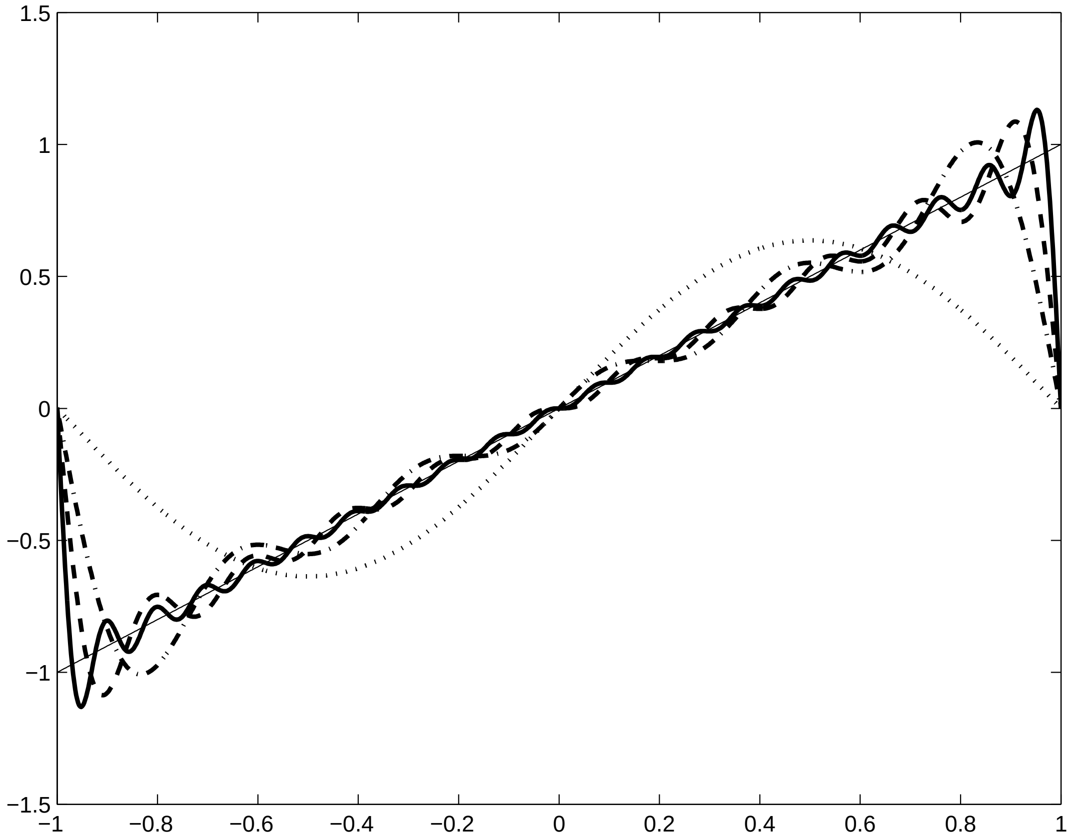

Figure 1: Plots (with $L = 1$) of the sawtooth function $f(x) = x$ (thin solid line) and the partial sums $f_1(x)$ (dots); $f_5(x)$ (dot-dashed); $f_{10}(x)$ (dashed); and $f_{20}(x)$ (solid).

If we substitute $x = 0$ and $L = 1$ into the series we get

$$\frac{\pi^2}{12} = 1 - \frac{1}{4} + \frac{1}{9} - \frac{1}{16} + \frac{1}{25} - \dots$$

Many such interesting formulae can be constructed using Fourier series (cf. more later!)

Finally, notice the coincidence of the term-by-term derivative of this Fourier series eq. (9) and the series in eq. (8). We now look into this property more carefully.

1.3 Integration and differentiation of Fourier series

Integration is always ok

Fourier series can always be integrated term-by-term. Suppose $f(x)$ is periodic with period $2L$ and satisfies the Dirichlet conditions so it has a Fourier series for $-L \leq x \leq L$:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \right].$$

It is then always valid to integrate term by term to get (here $-L \leq x \leq L$ and F is extended to all of $\mathbb{R}$ by periodicity)

$$\begin{aligned} F(x) \equiv \int_{-L}^{x} f(u)du &= \frac{a_0(x+L)}{2} + \sum_{n=1}^{\infty} \frac{a_n L}{n\pi} \sin\left(\frac{n\pi x}{L}\right) \\ &\quad + \sum_{n=1}^{\infty} \frac{b_n L}{n\pi} \left[(-1)^n - \cos\left(\frac{n\pi x}{L}\right) \right], \\ &= \frac{a_0 L}{2} + L \sum_{n=1}^{\infty} (-1)^n \frac{b_n}{n\pi} \\ &\quad - L \sum_{n=1}^{\infty} \frac{b_n}{n\pi} \cos\left(\frac{n\pi x}{L}\right) \\ &\quad + L \sum_{n=1}^{\infty} \left(\frac{a_n - (-1)^n a_0}{n\pi} \right) \sin\left(\frac{n\pi x}{L}\right), \end{aligned}$$

where we have used eq. (8).

Note that the first infinite series on RHS of the last equality above, forms part of the constant term in the Fourier series for $F(x)$. This infinite series is always guaranteed to converge – since b_n comes from a Fourier series we know that b_n is at worst $O(1/n)$ so $\sum(-1)^n b_n/n$ converges by comparison test with $\sum M/n^2$ for a suitable constant M.

It is to be expected that the convergence of the Fourier series for $F(x)$ will be faster (i.e. fewer terms will give a certain level of approximation) than for $f(x)$ due to the extra factor of $1/n$ making the coefficients decrease faster. This is unsurprising since integration is naturally a smoothing operation. Recall also that the Dirichlet conditions

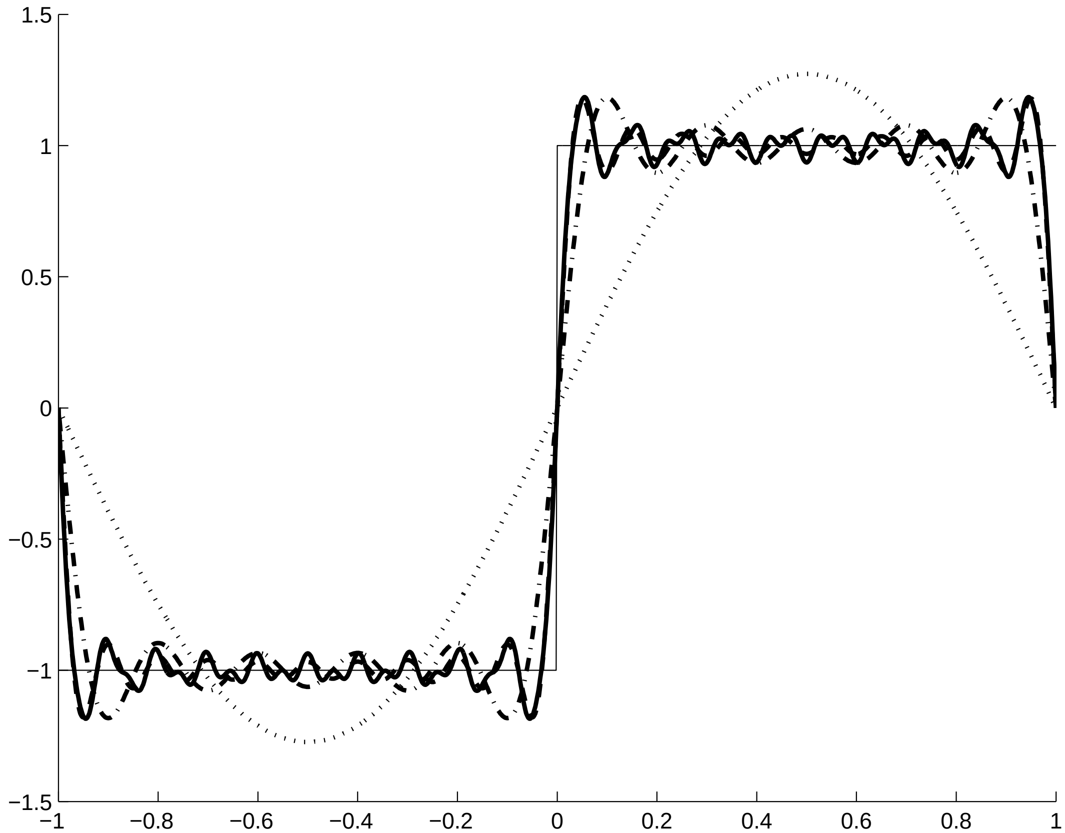

Figure 2: Plots of $f(x) = 1$ for $0 < x < 1$ and $f(x) = -1$ for $-1 < x < 0$ (thin solid line) and the partial sums $f_1(x)$ (dots); $f_5(x)$ (dot-dashed); $f_{10}(x)$ (dashed); and $f_{20}(x)$ (solid).

allow for finite jump discontinuities in the underlying function. But integration across such a jump leads to a continuous function, and $F(x)$ will always satisfy the Dirichlet conditions if $f(x)$ does.

Differentiation doesn't always work!

On the other hand, term-by-term differentiation of the Fourier series of a function is not guaranteed to yield a convergent Fourier series for the derivative! Consider this counter-example. Let $f(x)$ be a periodic function with period 2 such that $f(x) = 1$ for $0 < x < 1$ and $f(x) = -1$ for $-1 < x < 0$, as shown in the figure.

You can readily calculate (exercise!) its Fourier series to be

$$f(x) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{\sin([2n-1]\pi x)}{2n-1} \tag{10}$$

and formally differentiating term by term we get

$$f'(x) \overset{?}{=} 4 \sum_{n=1}^{\infty} \cos([2n-1]\pi x) \tag{11}$$

which is clearly divergent even though for our actual function we have $f'(x) = 0$ for all $x \neq 0$! The latter may look like a rather harmless function, but what about $f'(0)$? f' is *not defined* at $x = 0$ so f' *does not satisfy the Dirichlet conditions*. Why not just put in some value $f'(0) = c$ at the single point $x = 0$? e.g. the average of left and right limits, $c = 0$? Well, then consider the desired relationship $f(x) = f(-1) + \int_{-1}^{x} f'(t)dt$. For any finite c, $f(x)$ will remain at $f(-1)$ as x crosses $x = 0$ from below. To get the jump in $f(x)$ at $x = 0$, intuitively we'd need $f'(0)$ to introduce a finite area under the graph of f', but only over $x = 0$ with zero horizontal extent! i.e. we'd need $f'(0) = \infty$ with "$0 \cdot \infty = 1$"! Thus the operation of differentiation behaves badly (or rather most interestingly, cf later when we discuss the so-called Dirac delta function!) when we try to differentiate over a jump discontinuity, even if we have nice differentiable pieces on both sides.

So, when *can* we legitimately differentiate the Fourier series of a function term by term? Clearly it is not enough for f to satisfy the Dirichlet conditions (merely guaranteeing a Fourier series for f itself). It suffices for f to also not have any jump discontinuities (on $\mathbb{R}$) and we have the following result.

Theorem: Suppose f is *continuous* on $\mathbb{R}$ and has period $2L$ and satisfies the Dirichlet conditions on $(-L, L)$. Suppose further that f' satisfies the Dirichlet conditions. Then the Fourier series for f' can be obtained by term-by-term differentiation of the Fourier series for f. $\square$

To see this, note that the conditions imply that both f and f' *have* Fourier series:

$$\begin{aligned} f(x) &= \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right)\right], \\ f'(x) &= \frac{1}{2}A_0 + \sum_{n=1}^{\infty}\left[A_n \cos\left(\frac{n\pi x}{L}\right) + B_n \sin\left(\frac{n\pi x}{L}\right)\right]. \end{aligned}$$

and so

$$\begin{aligned} A_0 &= \frac{1}{L}\int_0^{2L} f'(x)\,dx = \frac{f(2L) - f(0)}{L} = 0 \text{ by periodicity,} \\ A_n &= \frac{1}{L}\int_0^{2L} f'(x)\cos\left(\frac{n\pi x}{L}\right)\,dx, \\ &= \frac{1}{L}\left[f(x)\cos\left(\frac{n\pi x}{L}\right)\right]_0^{2L} + \frac{n\pi}{L^2}\int_0^{2L} f(x)\sin\left(\frac{n\pi x}{L}\right)dx, \\ &= 0 + \frac{n\pi b_n}{L}. \end{aligned} \tag{12}$$

where we have again used periodicity and eqs. (7,6) for the Fourier coefficients. Similarly

$$B_n = \frac{-n\pi a_n}{L}$$

so the series for f' is obtained by term-by-term differentiation of the series for f. Note that the differentiation of f has been reduced to just simple multiplication of the Fourier coefficients by $\frac{n\pi}{L}$ (together with cross-relating the roles of a_n and b_n and adding in a minus sign for the B_n's).

1.4 Complex form of Fourier series

When dealing with sines and cosines it is often easier and more elegant to use complex exponentials via de Moivre's theorem

$$e^{i\theta} = \cos\theta + i\sin\theta$$

so

$$\begin{aligned} \cos\left(\frac{n\pi x}{L}\right) &= \frac{1}{2}\left(e^{\frac{in\pi x}{L}} + e^{-\frac{in\pi x}{L}}\right), \\ \sin\left(\frac{n\pi x}{L}\right) &= \frac{1}{2i}\left(e^{\frac{in\pi x}{L}} - e^{-\frac{in\pi x}{L}}\right) \end{aligned}$$

and our Fourier series becomes

$$\begin{aligned} \frac{f(x_+) + f(x_-)}{2} &= \frac{a_0}{2} + \sum_{n=1}^{\infty}\left[\frac{a_n}{2}\left(e^{\frac{in\pi x}{L}} + e^{-\frac{in\pi x}{L}}\right) + \frac{b_n}{2i}\left(e^{\frac{in\pi x}{L}} - e^{-\frac{in\pi x}{L}}\right)\right], \\ &= \sum_{-\infty}^{\infty} c_n e^{\frac{in\pi x}{L}}, \end{aligned} \tag{13}$$

where

$$\begin{aligned} c_n &= (a_n - ib_n)/2 \quad n > 0; \\ c_{-n} &= (a_n + ib_n)/2 \quad n > 0; \\ c_0 &= a_0/2. \end{aligned} \tag{14}$$

This is a neater (though completely equivalent) formulation. (These formulas all remain valid even if f is complex-valued, in which case the a_n's and b_n's are themselves complex).

We can work directly in this complex formulation by noting that the relevant complex exponentials are orthogonal functions:

$$(e^{\frac{im\pi x}{L}}, e^{\frac{in\pi x}{L}}) = \int_0^{2L} e^{\frac{in\pi x}{L}} e^{\frac{-im\pi x}{L}}\, dx = 2L\delta_{nm} \quad \text{for } m, n \in \mathbb{Z}. \tag{15}$$

Note the signs (i.e. complex conjugation) in the integral here! – in accordance with our definition of inner products for *complex* valued functions.

Using orthogonality, in the by now familiar way, we get from eq. (13):

$$c_m = \frac{1}{2L}\int_0^{2L} f(x) e^{\frac{-im\pi x}{L}}\, dx \qquad m \in \mathbb{Z}.$$

For *real*-valued functions f (most functions in this course) we immediately get $c_{-m} = c_m^*$ so we need only compute c_0 (which is real) and c_m for $m > 0$.

Example. (Differentiation rule revisited). Assuming we can differentiate the Fourier series term by term, in the complex representation we write

$$\begin{aligned} f(x) &= \sum_{n=-\infty}^{\infty} c_n e^{\frac{in\pi x}{L}}, \\ \frac{df}{dx} &= \sum_{n=-\infty}^{\infty} C_n e^{\frac{in\pi x}{L}} \end{aligned}$$

and the differentiation rule then gives the single simple formula:

$$C_n = \frac{in\pi}{L} c_n \quad \text{holding for all } n \in \mathbb{Z}.$$

1.5 Half-range series

Consider a function $f(x)$ defined **only** on the "half range" $0 \leq x \leq L$. It is possible to extend this function to the full range $-L \leq x \leq L$ (and then to a $2L$-periodic function) in two natural different ways, with different symmetries.

Fourier sine series: odd functions

The function $f(x)$ can be extended to be an **odd** function $f(-x) = -f(x)$ on $-L \leq x \leq L$, and then extended as a $2L$-periodic function. In this case, from eq. (7), $a_n = 0$ for all n and we get a **Fourier sine series** for f (note the range of integration):

$$\begin{aligned} \frac{f(x_+) + f(x_-)}{2} &= \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right); \\ b_n &= \frac{2}{L}\int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx. \end{aligned} \tag{16}$$

i.e. $f(x)$ on $[0, L]$ has been represented as a Fourier series with only sine terms.

Fourier cosine series: even functions

Alternatively, the function $f(x)$ can be extended to be an **even** function $f(-x) = f(x)$ on $-L \leq x \leq L$, and then extended as a $2L$-periodic function. In this case, from eq. (6), $b_n = 0$ for all n and we get a **Fourier cosine series** (note again the range of integration):

$$\begin{aligned} \frac{f(x_+) + f(x_-)}{2} &= \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right); \\ a_n &= \frac{2}{L}\int_0^L f(x) \cos\left(\frac{n\pi x}{L}\right) dx. \end{aligned} \tag{17}$$

which again represents f on $[0, L]$ but now as a Fourier series with only cosine terms.

1.6 Parseval's theorem for Fourier series

The integral of a squared periodic function (or squared modulus for complex functions) is often of interest in applications, e.g. representing the energy of a periodic signal

$$E = \int_0^{2L} |f(x)|^2 \, dx = (f, f). \tag{18}$$

Substituting the complex form of the Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{in\pi x}{L}}$$

and using the orthogonality property eq. (15) of the complex exponentials we immediately get

$$\int_0^{2L} |f(x)|^2\, dx = 2L \sum_{n=-\infty}^{\infty} |c_n|^2. \tag{19}$$

This result is called **Parseval's theorem**. Equivalently this can be expressed in terms of the a_n and b_n using eq. (14) as

$$\int_0^{2L} [f(x)]^2 dx = L \left[\frac{|a_0|^2}{2} + \sum_{n=1}^{\infty} (|a_n|^2 + |b_n|^2) \right] \tag{20}$$

i.e. the energy is obtained by adding together contributions from separate sinusoidal harmonics whose energies are proportional to their squared amplitudes. If f is a real-valued function, we can remove all the modulus signs in the above formula.

Remark: Parseval's formula can be interpreted as a kind of infinite dimensional version of Pythagoras' theorem (that the squared length of a vector is the sum of the squared components in any orthonormal basis). Indeed on $[-L, L]$ the following functions form an ortho*normal* set (i.e. pairwise orthogonal and each having norm 1):

$$\begin{cases} c_0 = 1/\sqrt{2L} \\ f_n(x) = \frac{1}{\sqrt{L}} \sin \frac{n\pi x}{L} \quad \text{for } n = 1, 2, \ldots \\ g_n(x) = \frac{1}{\sqrt{L}} \cos \frac{n\pi x}{L} \quad \text{for } n = 1, 2, \ldots \end{cases}$$

The Fourier series eq. (4) with these slightly rescaled basic functions becomes

$$f(x) = (\sqrt{\frac{L}{2}} a_0)\ c_0 + \sum_{n-1}^{\infty} \sqrt{L} a_n\ f_n(x) + \sqrt{L} b_n\ g_n(x)$$

and then Parseval's theorem eq. (20) is formally just Pythagoras' theorem in this infinite dimensional setting.
For a second interpretation of Parseval's formula, we start by viewing the Fourier series for f as a mapping M from functions f to doubly infinite sequences $\{c_n : n \in \mathbb{Z}\}$ of Fourier coefficients. Then viewing the latter as components of an infinite dimensional vector, Parseval's theorem eq. (19) states that the mapping M (up to an overall constant $2L$) is an *isometry* (i.e. length-preserving, according to natural notions of length on both sides).

Example. Consider again the sawtooth function $f(x) = x$ for $-L \le x \le L$. If we substitute eq. (8) into Parseval's formula eq. (20) we get

$$\int_{-L}^{L} x^2 dx \quad = \quad \frac{2L^3}{3} = L \sum_{m=1}^{\infty} \frac{4L^2}{m^2 \pi^2}$$

giving the nice formula

$$\frac{\pi^2}{6} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \ldots$$

Parseval's theorem is indeed commonly used to construct such tantalising equalities. As another example (exercise) Parseval's formula can be applied to eq. (9) to obtain

$$\sum_{m=1}^{\infty} \frac{1}{m^4} = \frac{\pi^4}{90}. \qquad (21)$$

2 STURM-LIOUVILLE THEORY

Sturm-Liouville (SL) theory is about the properties of a particular class of second order linear ODEs that arise very commonly in physical applications (as we'll see more later). Recall that in our study of Fourier series we intuitively viewed (complex-valued) functions on $[a, b]$ as vectors in an infinite dimensional vector space equipped with an inner product defined by

$$(f, g) = \int_a^b f^*(x) g(x) dx. \tag{22}$$

A fundamentally important feature was that the basic Fourier (trig or complex exponential) functions were orthogonal relative to this inner product and the set of them was *complete* in the sense that any (suitably well behaved) function could be expressed as an infinite series in terms of them.

In finite dimensional linear algebra of vectors with an inner product we have a very nice theory of *self-adjoint* or *Hermitian* matrices (that you saw in first year!) viz. their eigenvalues are real, eigenvectors belonging to different eigenvalues are orthogonal and we always have a complete set (i.e. a full basis) of orthonormal eigenvectors. SL theory can be viewed as a lifting of these ideas to the infinite dimensional setting, with vectors being replaced by functions (as before), matrices (i.e. linear maps on vectors) by linear second order differential operators, and we'll have a notion of self-adjointness for those operators. The basic formalism of Fourier series will reappear as a simple special case!

2.1 Revision of second order linear ODEs

Consider the general linear second-order differential equation

$$\mathcal{L}y(x) \;=\; \alpha(x)\frac{d^2}{dx^2}y + \beta(x)\frac{d}{dx}y + \gamma(x)y = f(x), \tag{23}$$

where α, β, γ are continuous, $f(x)$ is bounded, and α is nonzero (except perhaps at a finite number of isolated points), and $a \leq x \leq b$ (which may tend to $-\infty$ or $+\infty$).

The **homogeneous** equation $\mathcal{L}y = 0$ has two non-trivial linearly independent solutions $y_1(x)$ and $y_2(x)$ and its general solution is called the **complementary function**

$$y_c(x) = Ay_1(x) + By_2(x).$$

Here A and B are arbitrary constants. For the **inhomogeneous** or **forced** equation $\mathcal{L}y = f$ ($f(x)$ describes the **forcing**) it is usual to seek a **particular integral** solution y_p which is just any single solution of it. Then the general solution of eq. (23) is

$$y(x) = y_c(x) + y_p(x).$$

Finding a particular solutions can sometimes involve some inspired guesswork e.g. substituting a suitable guessed form for y_p with some free parameters which are then matched to make y_p satisfy the equation. However there are some more systematic ways of constructing particular integrals: (a) using the theory of so-called **Green's functions** that we'll study in more detail later, and (b) using SL theory, which also has other important uses too – later we will see how it can be used to construct solutions to *homogeneous* PDEs, especially in conjunction with the method of separation of variables, which reduces the PDE into a set of inter-related Sturm-Liouville ODE problems.

In physical applications (modelled by second order linear ODEs) where we want a unique solution, the constants A and B in the complementary function are fixed by imposing suitable **boundary conditions** (BCs) at one or both ends. Examples of such conditions include:
(i) Dirichlet boundary value problems: we specify y on the two boundaries e.g. $y(a) = c$ and $y(b) = d$;
(ii) Homogeneous BCs e.g. $y(a) = 0$ and $y(b) = 0$ (homogeneous conditions have the feature that if y_1 and y_2 satisfy them then so does $c_1y_1 + c_2y_2$ for any $c_1, c_2 \in \mathbb{R}$);
(iii) Initial value problems: y and y' are specified at $x = a$;
(iv) Asymptotic boundedness conditions e.g. $y \to 0$ as $x \to \infty$ for infinite domains;
etc.

2.2 Properties of self-adjoint matrices

As a prelude to SL theory let's recall some properties of (complex) N-dimensional vectors and matrices. If u and v are N-dimensional complex vectors, represented as *column* vectors of complex numbers then their inner product is

$$(u, v) = u^\dagger v$$

where the dagger denotes 'complex conjugate transpose' (so $u^\dagger$ is a row vector of the complex conjugated entries of u).

If A is any $N \times N$ complex matrix, its *adjoint* (or *Hermitian conjugate*) is $A^\dagger$ (i.e. complex conjugate transposed matrix) and A is *self-adjoint* or *Hermitian* if $A = A^\dagger$. There is a neater (more abstract..) way of defining adjoints: B is the adjoint of A if for all vectors u and v we have:

$$(u, Av) = (Bu, v) \tag{24}$$

(as you can easily check using the property that $(Bu)^\dagger = u^\dagger B^\dagger$). Note that this characterisation of the adjoint depends only on the notion of an inner product so we can apply it in any other situation where we have a notion of inner product (and you can probably imagine where this is leading!...)

Now let A be any self-adjoint matrix. Its eigenvalues λ_n and corresponding eigenvectors v_n are defined by

$$Av_n = \lambda_n v_n \tag{25}$$

and you should recall the following facts:
If A is self-adjoint then
(1) the eigenvalues λ_n are all real;

(2) if $\lambda_m \neq \lambda_n$ then corresponding eigenvectors are orthogonal $(v_m, v_n) = 0$;
(3) by rescaling the eigenvectors to have unit length we can always find an orthonormal basis of eigenvectors $\{v_1, \ldots, v_N\}$ so any vector w in $\mathbb{C}^N$ can be written as a linear combination of eigenvectors.
Note: it is possible for an eigenvalue λ to be degenerate i.e. having more than one linearly independent eigenvector belonging to it. For any eigenvalue, the set of all associated eigenvectors forms a vector subspace and for our orthogonal basis we choose an orthonormal basis of each of these subspaces. If λ is non-degenerate, the associated subspace is simply one-dimensional.
(4) A is non-singular iff all eigenvalues are nonzero.

The above facts give a neat way of solving the linear equation $Ax = b$ for unknown $x \in \mathbb{C}^N$, when A is nonsingular and self-adjoint. Let $\{v_1, \ldots, v_N\}$ be an orthonormal basis of eigenvectors belonging to eigenvalues $\lambda_1, \ldots, \lambda_N$ respectively. Then we can write

$$b = \sum \beta_i v_i \qquad x = \sum \xi_i v_i$$

where the $\beta_j = (v_j, b)$ (by orthonormality of the v_i) are known and ξ_j are the unknowns. Then

$$Ax = A \sum \xi_i v_i = \sum \xi_i A v_i = \sum \xi_i \lambda_i v_i = b = \sum \beta_i v_i. \tag{26}$$

Forming the inner product with v_j (for any j) gives $\xi_j \lambda_j = \beta_j$ so $\xi_j = \beta_j / \lambda_j$ and we get our solution $x = \sum \frac{\beta_j}{\lambda_j} v_j$. For this to work, we need that no eigenvalue is zero. If we have a zero eigenvalue i.e. a nontrivial solution of $Ax = 0$ then A is singular and $Ax = b$ either has no solution or a non-unique solution (depending on the choice of b).

2.3 Self-adjoint differential operators

Consider the general second order linear differential operator $\mathcal{L}$:

$$\mathcal{L}y = \alpha(x) \frac{d^2}{dx^2} y + \beta(x) \frac{d}{dx} y + \gamma(x) y$$

for $a \leq x \leq b$ (and α, β, γ are all real valued functions). In terms of the inner product eq. (22) of functions, we define $\mathcal{L}$ to be **self-adjoint** if

$$\begin{array}{rcl} (y_1, \mathcal{L}y_2) & = & (\mathcal{L}y_1, y_2) \\ \text{i.e.} \quad \int_a^b y_1^*(x)\, \mathcal{L}y_2(x)\, dx & = & \int_a^b (\mathcal{L}y_1(x))^*\, y_2(x)\, dx \end{array} \tag{27}$$

for all functions y_1 and y_2 *that satisfy some specified boundary conditions*. It is important to note that self-adjointness is not a property of $\mathcal{L}$ alone but also incorporates a specification of boundary conditions restricting the class of functions being considered i.e. we are also able to vary the underlying space on which $\mathcal{L}$ is being taken to act. This feature arises naturally in many applications.

Note that $(\mathcal{L}y)^* = \mathcal{L}(y^*)$ since we are taking $\mathcal{L}$ to have real coefficient functions α, β, γ. Furthermore if we work with real-valued functions y then the complex conjugations in eq. (27) can be omitted altogether.

Eigenfunctions of $\mathcal{L}$ and weight functions

Let $w(x)$ be a real-valued non-negative function on $[a, b]$ (with at most a finite number of zeroes). A function y (satisfying the BCs being used) is an **eigenfunction** for the self-adjoint operator $\mathcal{L}$ **with eigenvalue** λ **and weight function** w if

$$\mathcal{L}y(x) = \lambda w(x)y(x). \tag{28}$$

Note that this is formally similar to the matrix eigenvector equation eq. (25) but here we have the extra ingredient of the weight function. Equations of this form (with various choices of w) occur frequently in applications. (In the theory developed below, the appearance of w could be eliminated by making the substitution $\tilde{y} = \sqrt{w}y$ and replacing $\mathcal{L}y$ by $\frac{1}{\sqrt{w}}\mathcal{L}(\frac{\tilde{y}}{\sqrt{w}})$ but it is generally simpler to work with w in place, as done in all textbooks, and express our results correspondingly).

Eigenvalues and eigenfunctions of self-adjoint operators enjoy a series of properties that parallel those of self-adjoint matrices.

Property 1: the eigenvalues are always real.

Property 2: eigenfunctions y_1 and y_2 belonging to different eigenvalues $\lambda_1 \neq \lambda_2$ are always orthogonal *relative to the weight function* w:

$$\int_a^b w(x)y_1^*(x)y_2(x)\,dx = 0. \tag{29}$$

Thus by rescaling the eigenfunctions we can form an orthonormal set

$$Y(x) = y(x)/\sqrt{\int_a^b w|y|^2 dx}.$$

Remark: Note that the inner product eq. (27), used to define self-adjointness, has no weight function (i.e. $w = 1$ there) whereas the eigenfunctions are orthogonal only if we incorporate the weight w from the eigenvalue equation eq. (28) into the inner product. Alternatively we may think of the functions $\sqrt{w}y_i$ as being orthogonal relative to the unweighted inner product.

Remark: We may always take our eigenfunctions to be *real-valued* functions. This is because in eq. (28), λ, w and the coefficient functions of $\mathcal{L}$ are all real. Hence by taking the complex conjugate of this equation we see that if y is an eigenfunction belonging to λ then so is y^*. Hence if the eigenvalue is nondegenerate, y must be real (i.e. $y = y^*$). For degenerate eigenvalues we can always take the two real functions $(y + y^*)$ and $(y - y^*)/i$ as our eigenfunctions, with the same span.
In this course *we will always assume that our eigenfunctions are real-valued*, so we can omit the complex conjugation in the weighted inner product expressions such as eq. (30).

Property 3: There is always a countable infinity of eigenvalues $\lambda_1, \lambda_2, \lambda_3, \ldots$ and the corresponding set of (normalised) eigenfunctions $Y_1(x), Y_2(x), \ldots$ forms a **complete basis** for functions on $[a, b]$ satisfying the BCs being used i.e. any such function f can be expressed as

$$f(x) = \sum_{n=1}^{\infty} A_n Y_n(x)$$

and property 2 gives

$$A_n = \int_a^b w(x) f(x) Y_n(x)\, dx.$$

(Don't forget here to insert the weight function into the "inner product" integral!)

Remark: the *discreteness* of the series of eigenvalues is a remarkable feature here. The eigenvalue equation itself appears to involve no element of discreteness, and this can be intuitively attributed to the imposition of *boundary conditions*, as illustrated in the next example below. □

Demonstration of the completeness property 3 is beyond the scope of this course, but properties 1 and 2 can be seen using arguments similar to those used in the finite dimensional case, for self-adjoint matrices. Introduce the notation

$$(f,g) = \int_a^b f^* g\, dx \qquad (f,g)_w = \int_a^b w f^* g\, dx$$

so (since w is real)

$$(wf, g) = (f, wg) = (f, g)_w. \tag{30}$$

Now since $\mathcal{L}$ is self-adjoint we have

$$(y_1, \mathcal{L} y_2) = (\mathcal{L} y_1, y_2) \quad \text{for any } y_1, y_2 \text{ satisfying the BCs.} \tag{31}$$

If also y_1, y_2 are eigenfunctions belonging to eigenvalues λ_1, λ_2 respectively i.e. $\mathcal{L} y_i = \lambda_i w y_i$, then eq. (31) gives $(\lambda_1 w y_1, y_2) = (y_1, \lambda_2 w y_2)$ and applying eq. (30) we get $\lambda_1^*(y_1, y_2)_w = \lambda_2 (y_1, y_2)_w$ i.e.

$$(\lambda_1^* - \lambda_2)(y_1, y_2)_w = 0. \tag{32}$$

Now taking $y_1 = y_2$ with $\lambda_1 = \lambda_2 = \lambda$, eq.(32) gives $\lambda^* - \lambda = 0$ (as $(y,y)_w \neq 0$ for $y \neq 0$) i.e. any eigenvalue λ must be real. Finally taking $\lambda_1 \neq \lambda_2$ we have $\lambda_1^* - \lambda_2 = \lambda_1 - \lambda_2 \neq 0$ so eq. (32) gives $(y_1, y_2)_w = 0$, completing the proof of properties 1 and 2. □

Let's now illustrate these ideas with the simplest example.

Example (Fourier series again!) Consider

$$\mathcal{L} = \frac{d^2}{dx^2} \text{ on } 0 \leq x \leq L$$

i.e. the coefficient functions are $\alpha(x) = 1, \beta(x) = \gamma(x) = 0$. We impose the homogeneous boundary conditions:

$$y(0) = 0 \quad y(L) = 0$$

and we take the weight function to be simply

$$w(x) = 1.$$

We will work only with real-valued functions (and hence omit all complex conjugations).

Is $\mathcal{L}$ self-adjoint? Well, we just need to calculate

$$(y_1, \mathcal{L}y_2) = \int_0^L y_1 y_2''\, dx \quad \text{and} \quad (\mathcal{L}y_1, y_2) = \int_0^L y_1'' y_2\, dx$$

Integrating by parts twice we get

$$\int_0^L y_2 y_1''\, dx = [y_2 y_1']_0^L - \int_0^L y_2' y_1'\, dx = [y_2 y_1' - y_2' y_1]_0^L + \int_0^L y_2'' y_1\, dx$$

so

$$(\mathcal{L}y_1, y_2) - (y_1, \mathcal{L}y_2) = [y_2 y_1' - y_2' y_1]_0^L.$$

With our BCs we see that RHS $= 0$ so *with this choice of BCs* $\mathcal{L}$ is self-adjoint.

Let's calculate its eigenvalues and eigenfunctions:

$$\mathcal{L}y = -\lambda w y = -\lambda y$$

(the minus sign on RHS being for convenience, just a relabelling of the λ values) i.e.

$$y'' = -\lambda y \quad \text{with} \quad y(0) = y(L) = 0.$$

For $\lambda \leq 0$ the BCs give $y(x) = 0$. For $\lambda > 0$ the solutions are well known to be

$$y_n = \sin \frac{n\pi x}{L} \qquad \lambda_n = \frac{n^2\pi^2}{L^2}.$$

Properties 2 and 3 then reproduce the theory of half-range Fourier sine series. You can easily check that if we had instead taken the same $\mathcal{L}$ but on $[-L, L]$ with periodic boundary conditions $y(-L) = y(L)$ and $y'(-L) = y'(L)$ (and weight function $w(x) = 1$ again) then $\sin n\pi x/L$ and $\cos n\pi x/L$ would be (real) eigenfunctions belonging to the (now degenerate) eigenvalues $n^2\pi^2/L^2$ and properties 2 and 3 give the formalism of full range Fourier series (at least as applicable to suitably differentiable functions).

2.4 Sturm-Liouvlle theory

The above example is the simplest case of a so-called **Sturm-Liouville equation**. Consider again the general second order linear differential operator (with new names for the coefficient functions, as often used in texts)

$$\mathcal{L}y \equiv p(x)y'' + r(x)y' + q(x)y \tag{33}$$

where p, q, r are real-valued functions on $a \leq x \leq b$. How can we choose the functions p, q, r (and also associated BCs) to make $\mathcal{L}$ self-adjoint? An important way is the following. We will require that

$$r(x) = \frac{dp}{dx} \tag{34}$$

so we can write $\mathcal{L}$ as

$$\mathcal{L}y = (py')' + qy.$$

Can $\mathcal{L}$ be self-adjoint? (recalling that we still need to specify some BCs!). Well, integrating by parts twice (as in the above example, and taking all functions to be real) you can readily verify that

$$\begin{aligned}(y_1, \mathcal{L}y_2) - (\mathcal{L}y_1, y_2) &= \int_a^b y_1[(py_2')' + qy_2] - y_2[(py_1')' + qy_1]\,dx \\ &= [p(y_1y_2' - y_2y_1')]_a^b = \left[p \det \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix}\right]_a^b\end{aligned}$$

$\mathcal{L}$ will be self-adjoint if we impose BCs making the above boundary term combination zero. The following are examples of such BCs:
(i) $y = 0$ at $x = a, b$;
(ii) $y' = 0$ at $x = a, b$;
(iii) $y + ky' = 0$ at $x = a, b$ (for any constants k which may differ at $x = a$ and $x = b$);
(iv) periodic BCs: $y(a) = y(b)$ and $y'(a) = y'(b)$;
(v) $p = 0$ at $x = a, b$ (the endpoints of the interval are then singular points of the ODE).

If $w(x)$ is any weight function then the corresponding eigenfunction equation

$$\mathcal{L}y = (py')' + qy = -\lambda wy$$

(with any choice of BCs making $\mathcal{L}$ self-adjoint) is called a **Sturm-Liouville equation**. Such equations arise naturally in many applications (we'll see some in section 2) and the eigenfunctions/values are then guaranteed to satisfy all the extremely useful properties 1,2,3 above. The Fourier series example above corresponds to the simplest non-trivial case of an SL equation (with $p(x) = 1, q(x) = 0$ and $w(x) = 1$).

Reducing general second order $\mathcal{L}$'s to SL form
The SL condition eq. (34) viz. that $r = p'$, on the coefficients of a general second order operator appears to be a nontrivial restriction, but in fact, any second order differential operator $\mathcal{L}$ as in eq. (33) can be re-cast into the SL form as follows.

Consider the general eigenfunction equation

$$py'' + ry' + qy = -\lambda wy \qquad a \leq x \leq b \tag{35}$$

(with weight w non-negative but r not necessarily equal to p'). Consider multiplying through by some function $F(x)$. The new coefficients of y'' and y' are Fp and Fr respectively and we want to choose F (then called the integrating factor) to have

$$(Fr) = (Fp)' \quad \text{i.e.} \quad pF' = (r - p')F$$

so

$$F(x) = \exp \int^x \left(\frac{r - p'}{p}\right) dx.$$

Then eq.(35) takes the SL form

$$[F(x)p(x)y']' + F(x)q(x)y = -\lambda F(x)w(x)y$$

with a new weight function $F(x)w(x)$ (which is still non-negative since $F(x)$ is a real exponential and hence always positive) and new coefficient functions Fp and Fq.

Example. (An SL equation with integrating factor and non-trivial weight function)

Consider the eigenfunction/eigenvalue equation on $[0, \pi]$:

$$\mathcal{L}y = y'' + y' + \frac{1}{4}y = -\lambda y$$

with boundary conditions

$$y = 0 \text{ at } x = 0 \qquad \text{and} \qquad y - 2y' = 0 \text{ at } x = \pi.$$

This is not in SL form since $p(x) = 1$ and $r(x) = 1 \neq p'(x)$. But the integrating factor is easily calculated:

$$F = \exp \int^x \frac{r - p'}{p}\, dx = e^x.$$

Multiplying through by this F gives the self-adjoint form (noting also the form of the given BCs!):

$$\frac{d}{dx}\left(e^x \frac{dy}{dx}\right) + \frac{e^x}{4}y = -\lambda e^x y$$

(and we can view $-\lambda$ as the eigenvalue).

To solve for the eigenfunctions it is easier here to use the original form of the equation (second order linear, *constant* coefficients) using standard methods (i.e. substitute $y = e^{\sigma x}$ giving $\sigma^2 + \sigma + \frac{1}{4} + \lambda = 0$ so $\sigma = -\frac{1}{2} \pm i\sqrt{\lambda}$) to obtain

$$y(x) = Ae^{-x/2} \cos \mu x + Be^{-x/2} \sin \mu x$$

where we have written $\mu = \sqrt{\lambda}$ (with $\mu \geq 0$) and A, B are arbitrary constants of integration.

The first BC requires $A = 0$ and then the second BC gives the transcendental equation (as you should check):

$$\tan \mu\pi = \mu. \tag{36}$$

Now to study the latter condition, in the positive quadrant of an xy plane imagine plotting the 45° line $y = x$ and the graph of $y = \tan \pi x$. The line crosses each branch of the tan function once giving an infinite sequence $\mu_1, \mu_2, \ldots$ of increasing solutions of eq. (36). As $n \to \infty$ (i.e. large x and y values in the plane) these crossing points approach the vertical asymptotes of the $\tan \pi x$ function, which are at $x\pi = (2n + 1)\pi/2$ so we see that $\mu_n \to (2n + 1)/2$ as $n \to \infty$ i.e. the eigenvalues have asymptotic form $\lambda_n \approx (2n+1)^2/4$. The associated eigenfunctions are proportional to $y_n(x) = e^{-x/2} \sin \mu_n x$. They are orthogonal if the correct weight function e^x is used:

$$\int_0^\pi e^x y_m(x) y_n(x)\, dx = 0 \quad \text{if } m \neq n$$

as you could verify by a direct integration (and you will need to use the special property eq. (36) of the μ_n values.) □

2.5 Parseval's identity and least square approximations

Looking back at Parseval's theorem for Fourier series we see that its derivation depends only on the *orthogonality* of the Fourier functions and not their particular (e.g. trig) form. Hence we can obtain a similar Parseval formula associated to any complete set of orthogonal functions, such as our SL eigenfunctions. Indeed let $\{Y_1(x), Y_2(x), \ldots\}$ be a complete orthonormal set of functions relative to an inner product with weight function w

$$\int_a^b wY_iY_j\,dx = \delta_{ij} \tag{37}$$

and suppose that

$$f(x) = \sum_{n=1}^{\infty} A_nY_n(x) \qquad A_n = \int_a^b wY_mf\,dx \tag{38}$$

(for simplicity we're assuming here that f and all Y_n's are real functions). Using the series for f and the orthogonality conditions we readily get

$$\int_a^b wf^2\,dx = \int_a^b w(\sum A_iY_i)(\sum A_jY_j)\,dx = \sum_{n=1}^{\infty} A_n^2.$$

Finally, it is possible to establish that the representation of a function in an eigenfunction expansion is the "best possible" representation in a certain well-defined sense. Consider the partial sum

$$S_N(x) = \sum_{n=1}^{N} A_nY_n(x),$$

The mean square error involved in approximating $f(x)$ by $S_N(x)$ is

$$\epsilon_N = \int_a^b w[f - S_N(x)]^2 dx.$$

How does this error depend on the coefficients A_m? Viewing the A_m's as variables we have

$$\begin{aligned}
\frac{\partial}{\partial A_m}\epsilon_N &= -2\int_a^b w[f - \sum_{n=1}^{N} A_nY_n]Y_m dx, \\
&= -2\int_a^b wfY_m dx + 2\sum_{n=1}^{N} A_n \int_a^b wY_mY_n dx, \\
&= -2A_m + 2A_m = 0,
\end{aligned}$$

once again using eqs. (37,38). Therefore the actual SL coefficients extremize the error in a mean square sense (in fact *minimise* it since $\frac{\partial^2\epsilon_N}{\partial A_m^2} = \int_a^b wY_mY_m\,dx > 0$), and so give the 'best' partial sum representation of a function is in terms of any (partial) eigenfunction expansion. This property is important computationally, where we want the best approximation within given resources.

2.6 SL theory and inhomogeneous problems

For systems of linear equations $Ax = b$ whose coefficient matrix was self-adjoint, we described a method of solution that utilised the eigenvectors of A – look back at eq. (26) *et. seq.* The same ideas may be applied in the context of self-adjoint differential operators and their eigenfunctions. Consider a general inhomogeneous (or forced) equation

$$\mathcal{L}y(x) = f(x) = wF(x) \tag{39}$$

where $\mathcal{L}$ on $[a, b]$ (with specified BCs) is self-adjoint, and we have also introduced a weight function w.

Mimicking the development of eq. (26), let $\{Y_n(x)\}$ be a complete set of eigenfunctions of $\mathcal{L}$ that are orthonormal relative to the weight function w:

$$\mathcal{L}Y_n = \lambda_n w Y_n \qquad \int_a^b wY_mY_n\,dx = \delta_{mn}$$

and (assuming that F can be expanded in the eigenfunctions) write

$$F(x) = \sum A_nY_n \qquad y(x) = \sum B_nY_n$$

where $A_n = \int_a^b wY_nF\,dx$ are known and B_n are the unknowns. Substituting these into eq. (39) gives

$$\mathcal{L}y = \sum B_n\lambda_n wY_n = w\sum A_nY_n.$$

Multiplying by Y_m and integrating from a to b immediately gives $B_m\lambda_m = A_m$ (by orthonormality of the Y_n's) and so we obtain the solution

$$y(x) = \sum_{n=1}^{\infty} \frac{A_n}{\lambda_n} Y_n(x). \tag{40}$$

Here we must assume that all eigenvalues λ_n are *non-zero*.

Example. In some applications, when a system modelled by a homogeneous equation

$$\mathcal{L}y = (py')' + qy = 0$$

is subjected to forcing, the function q develops a weighted linear term and we get

$$\tilde{\mathcal{L}}y = (py')' + (q + \mu w)y = f$$

where w is a weight function and μ is a given fixed constant. This occurs for example in the analysis of a vibrating non-uniform elastic string with fixed endpoints; $p(x)$ is the mass density along the string and μ, f depend on the applied driving force.

The eigenfunction equation for $\tilde{\mathcal{L}}$ (with weight function w, eigenvalues λ) is

$$\tilde{\mathcal{L}}y = \mathcal{L}y + \mu wy = \lambda wy.$$

Hence we easily see that the eigenfunctions Y_n of $\tilde{\mathcal{L}}$ are those of $\mathcal{L}$ but with eigenvalues $(\lambda_n - \mu)$ where λ_n are the eigenvalues of $\mathcal{L}$, and our formula eq. (40) above gives

$$y(x) = \sum_{n=1}^{\infty} \frac{A_n}{(\lambda_n - \mu)} Y_n(x).$$

This derivation is valid only if μ does not coincide with any eigenvalue λ_n. If μ does coincide with an eigenvalue then this method fails and (as in the finite dimensional matrix case) the solution becomes either non-unique or non-existent, depending on the choice of RHS function f.

2.7 The notion of a Green's function

Let us look a little more closely at the structure of the solution formula eq. (40). Substituting $A_n = \int_a^b w(\xi)Y_n(\xi)F(\xi)\,dx$ and interchanging the order of summation and integration we get

$$y(x) = \int_a^b \sum_{n=1}^{\infty} \frac{Y_n(x)Y_n(\xi)}{\lambda_n} w(\xi)F(\xi)\,d\xi \tag{41}$$

i.e.

$$y(x) = \int_a^b G(x;\xi)f(\xi)\,d\xi \tag{42}$$

where we have reinstated $f = Fw$ and introduced the **Green's function** G defined by

$$G(x;\xi) = \sum_{n=1}^{\infty} \frac{Y_n(x)Y_n(\xi)}{\lambda_n}. \tag{43}$$

Note that the Green's function depends only on $\mathcal{L}$ (i.e. its eigenfunctions and eigenvalues) and not the forcing function f. It also depends the boundary conditions, that are needed to make $\mathcal{L}$ self-adjoint and used in the construction of the eigenfunctions. Via eq. (42), it provides the solution of $\mathcal{L}y = f$ for any forcing term.

By analogy with "$Ax = b \Rightarrow x = A^{-1}b$" we can think of "integration against G" in eq. (42) as an expression of a formal inverse "$\mathcal{L}^{-1}$" of the linear differential operator $\mathcal{L}$:

$$\mathcal{L}y = f \qquad \Rightarrow \qquad y = \int_a^b G(x;\xi)f(\xi)\,d\xi.$$

This notion of a Green's function and its associated integral operator inverting a differential operator, is a very important construct and we'll encounter it again later in more general contexts, especially in solving inhomogeneous boundary value problems for PDEs.