Part IB — Methods

Based on lectures by Dr E P Shellard and notes by third sgames.co.uk ${\it Michaelmas}~2022$

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§1 Fourier Series

§1.1 Periodic Functions

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Definition 1.1 (Periodic function)
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A function f(x) is **periodic** if f(x+T)=f(x) for all x, where T is the *period*.

For example, simple harmonic motion is periodic. In space, we consider the wavelength $\lambda = \frac{2\pi}{k}$, and the (angular) wave number k is defined conversely by $k = \frac{2\pi}{\lambda}$.

Consider the set of functions

$$g_n(x) = \cos \frac{n\pi x}{L}; \quad h_n(x) = \sin \frac{n\pi x}{L}$$

where $n \in \mathbb{N}$. These functions are periodic on the interval $0 \le x < 2L$ with period T = 2L. Recall that

$$\cos A \cos B = \frac{1}{2}(\cos(A - B) + \cos(A + B));$$

$$\sin A \sin B = \frac{1}{2}(\cos(A - B) - \cos(A + B));$$

$$\sin A \cos B = \frac{1}{2}(\sin(A - B) + \sin(A + B))$$

Definition 1.2 (Inner product)

We define the **inner product** for two periodic functions f, g on the interval $0 \le x < 2L$.

$$\langle f, g \rangle = \int_0^{2L} f(x)g(x) \, \mathrm{d}x^a$$

The functions g_n and h_n are mutually orthogonal on the interval [0, 2L) with respect to the inner product above.

$$\langle h_n, h_m \rangle = \int_0^{2L} \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx$$

$$= \frac{1}{2} \int_0^{2L} \left(\cos \frac{(n-m)\pi x}{L} - \cos \frac{(n+m)\pi x}{L} \right) dx$$

$$= \frac{1}{2} \frac{L}{\pi} \left[\frac{1}{n-m} \sin \frac{(n-m)\pi x}{L} - \frac{1}{n+m} \sin \frac{(n+m)\pi x}{L} \right]_0^{2L}$$

$$= 0 \text{ when } n \neq m$$

If n = m, we have

$$\langle h_n, h_n \rangle = \int_0^{2L} \sin^2 \frac{n\pi x}{L} \, \mathrm{d}x = \frac{1}{2} \int_0^{2L} \left(1 - \cos \frac{2\pi nx}{L} \right) \, \mathrm{d}x = L \quad (n \neq 0)$$

Thus,

$$\langle h_n, h_m \rangle = \begin{cases} L\delta_{nm} & n, m \neq 0 \\ 0 & nm = 0 \end{cases}$$
 (1)

Similarly, we can show

$$\langle g_n, g_m \rangle = \begin{cases} L\delta_{nm} & n, m \neq 0 \\ 0 & \text{exactly one of } m, n \text{ is zero} \\ 2L & n, m = 0 \end{cases}$$
 (2)

^aWe will generalise this definition later when we use other eigen functions.

and

$$\langle h_n, g_m \rangle = 0 \tag{3}$$

Now, we assert that $\{g_n, h_n\}$ form a complete orthogonal set; they span the space of all 'well-behaved' periodic functions of period 2L. Further, the set $\{g_n, h_n\}$ is linearly independent.

§1.2 Definition of Fourier series

Since g_n, h_n span the space of 'well-behaved' periodic functions of period 2L, we can express any such function as a sum of such eigenfunctions.

Definition 1.3 (Fourier series)

The **Fourier series** (FS) of f is

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

where a_n, b_n are constants such that the right hand side is convergent for all x where f is continuous.^a

At a discontinuity x, the Fourier series approaches the midpoint of the supremum and infimum of the function in a close neighbourhood of x. That is, we replace the left hand side with

$$\frac{1}{2}f(x_{+}) + \frac{1}{2}f(x_{-})$$

Let m > 0, and consider taking the inner product $\langle h_m, f \rangle$ and substituting the Fourier series of f.

$$\langle h_m, f \rangle = \int_0^{2L} \sin \frac{m\pi x}{L} f(x) dx$$

$$= \int_0^{2L} \sin \frac{m\pi x}{L} \left(\frac{1}{2} a_0 + \sum_{n=1}^{\infty} a_n \cos \frac{n\pi x}{L} + \sum_{n=1}^{\infty} b_n \sin \frac{n\pi x}{L} \right) dx \text{ by substituting eq. (4)}$$

$$= \langle h_m, b_m h_m \rangle \text{ by orthogonality relations eqs. (1) to (3)}$$

$$= Lb_m$$

Thus,

$$b_n = \frac{1}{L} \langle h_n, f \rangle = \frac{1}{L} \int_0^{2L} \sin \frac{n\pi x}{L} f(x) dx$$

$$a_n = \frac{1}{L} \langle g_n, f \rangle = \frac{1}{L} \int_0^{2L} \cos \frac{n\pi x}{L} f(x) dx$$
(5)

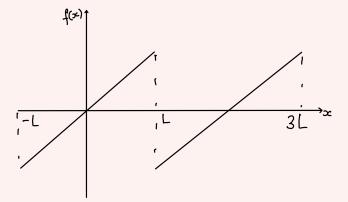
^aNote does not require differentiability unlike a Taylor series.

Note. • Note this includes the a_0 case so $\frac{1}{2}a_0$ is the average of the function.

- Note further that we may integrate over any range as long as the total length is one period, 2L. Notably, we may integrate over the interval [-L, L].
- Think of FS as a decomposition into harmonics. Simplest FS are sine and cosine function, e.g. pure mode $\sin \frac{3\pi x}{L}$, has $b_3 = 1, b_n = 0 \ \forall \ n \neq 3$.

Example 1.1 (Sawtooth wave)

Consider the sawtooth wave; defined by f(x) = x for $x \in [-L, L)$ and periodic elsewhere.



Here, $a_n = \frac{1}{L} \int_{-L}^{L} x \cos \frac{n\pi x}{L} dx = 0$ as x odd and \cos is even.

$$b_n = \frac{1}{L} \int_{-L}^{L} x \sin \frac{n\pi x}{L} dx$$

$$= \frac{2}{L} \int_{0}^{L} x \sin \frac{n\pi x}{L} dx \text{ as the function we are integrating is even}$$

$$= \frac{-2}{n\pi} \left[x \cos \frac{n\pi x}{L} \right]_{0}^{L} + \frac{2}{n\pi} \int_{0}^{L} \cos \frac{n\pi x}{L} dx$$

$$= \frac{-2L}{n\pi} \cos n\pi + \frac{2L}{(n\pi)^2} \sin n\pi$$

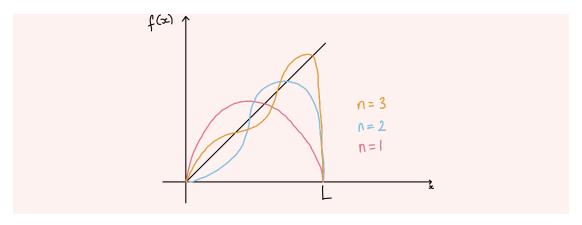
$$= \frac{2L}{n\pi} (-1)^{n+1}$$

So the sawtooth FS is

$$f(x) = \frac{2L}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin \frac{n\pi x}{L}$$

$$= \frac{2L}{\pi} \left(\sin \frac{\pi x}{L} - \frac{1}{2} \sin \frac{2\pi x}{L} + \frac{1}{3} \sin \frac{3\pi x}{L} + \dots \right)$$
(6)

which is slowly convergent.



Note. As $n \to \infty$

- 1. FS approx improves (convergent when cts)
- 2. FS \rightarrow 0 at x = L i.e. midpoint of discontinuity
- 3. FS has a persistent overshoot at x=L (approx 9% knows as Gibbs phenomenon, see Sheet 1, Q5).

§1.3 Dirichlet conditions

The Dirichlet conditions are sufficiency conditions for a "well-behaved" function, that will imply the existence of a unique Fourier series.

Theorem 1.1

If f(x) is a bounded periodic function of period 2L with a finite number of minima, maxima and discontinuities in [0, 2L), then the Fourier series converges to f at all points at which f is continuous, and at discontinuities the series converges to the midpoint.

Note.

- 1. These are some relatively weak conditions for convergence, compared to Taylor series. However, this definition still eliminates pathological functions such as $\frac{1}{x}$, $\sin \frac{1}{x}$, $\mathbb{1}(\mathbb{Q})$ and so on.
- 2. The converse is not true; for example, $\sin \frac{1}{x}$ does in fact have a Fourier series.
- 3. The proof is difficult and will not be given.

The rate of convergence of the Fourier series depends on the smoothness of the function.

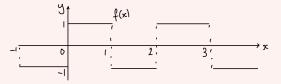
Theorem 1.2

If f(x) has continuous derivatives up to a pth derivative which is discontinuous, then the Fourier series converges with order $O(n^{-(p+1)})$ as $n \to \infty$.

Example 1.2 (p = 0)

Consider the square wave (Sheet 1, Q5)

$$f(x) = \begin{cases} 1 & 0 \le x < 1 \\ -1 & -1 \le x < 0 \end{cases}$$



Then the Fourier series is

$$f(x) = 4\sum_{m=1}^{\infty} \frac{\sin(2m-1)\pi x}{(2m-1)\pi}$$

Example 1.3 (p = 1)

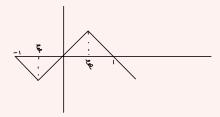
Consider the general 'see-saw' wave, defined by

$$f(x) = \begin{cases} x(1-\xi) & 0 \le x < \xi \\ \xi(1-x) & \xi \le x < 1 \end{cases}$$

and defined as an odd function for $-1 \le x < 0$. The Fourier series is

$$f(x) = 2\sum_{m=1}^{\infty} \frac{\sin n\pi \xi \sin n\pi x}{(n\pi)^2}$$

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For instance, if $\xi = \frac{1}{2}$, we can show that

$$f(x) = 2\sum_{m=1}^{\infty} (-1)^{m+1} \frac{\sin(2m-1)\pi x}{((2m-1)\pi)^2}$$

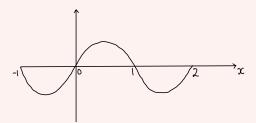
Example 1.4 (p = 2)

Let

$$f(x) = \frac{1}{2}x(1-x)$$

for $0 \le x < 1$, and defined as an odd function for $-1 \le x < 0$. We can show that

$$f(x) = 4\sum_{n=1}^{\infty} \frac{\sin(2m-1)\pi x}{((2m-1)\pi)^3}$$



 $[^]a\mathrm{This}$ is an important exercise you should do at home.

Example 1.5 (p = 3)

 $Consider^a$

$$f(x) = (1 - x^2)^2$$

with Fourier series

$$a_n = O\left(\frac{1}{n^4}\right)$$

§1.4 Integration of FS

It is always valid to take the integral of a Fourier series term by term. Defining $F(x) = \int_{-L}^{x} f(x) dx$, we can show that F satisfies the Dirichlet conditions if f does. For instance, a jump discontinuity becomes continuous in the integral.

§1.5 Differentiation

Differentiating term by term is not always valid. For example, consider the square wave above:

$$f(x) \stackrel{?}{=} 4 \sum_{m=1}^{\infty} \cos(2m-1)\pi x$$

which is an unbounded series (consider x = 0).

Theorem 1.3

If f(x) is continuous and satisfies the Dirichlet conditions, and f'(x) also satisfies the Dirichlet conditions, then f'(x) can be found term by term by differentiating the Fourier series of f(x).

Example 1.6

We can differentiate the see-saw function with $\xi = \frac{1}{2}$, even though the derivative is not continuous. The result is an offset square wave, or by mapping $x \mapsto x + \frac{1}{2}$ we recover the original square wave.

^aSheet 1, Q1

§1.6 Parseval's theorem

Parseval's theorem relates the integral of the square of a function with the sum of the squares of the function's Fourier series coefficients.

Theorem 1.4

Suppose f has Fourier coefficients a_i, b_i . Then

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

We can remove cross terms, since the basis functions are orthogonal. eqs. (1) to (3)

$$= \int_0^{2L} \left[\frac{1}{4} a_0^2 + \sum_{n=1}^\infty a_n^2 \cos^2 \frac{n\pi x}{L} + \sum_{n=1}^\infty b_n^2 \sin^2 \frac{n\pi x}{L} \right] dx$$

$$= L \left[\frac{1}{2} a_0^2 + \sum_{n=1}^\infty (a_n^2 + b_n^2) \right]$$
(7)

This is also called the completeness relation: the left hand side is greater than or equal to the right hand side if any of the basis functions are missing.

Example 1.7

Let us apply Parseval's theorem to the sawtooth wave.

$$\int_{-L}^{L} [f(x)]^2 dx = \int_{-L}^{L} x^2 dx = \frac{2}{3}L^3$$

The right hand side gives

$$L\sum_{n=1}^{\infty} \frac{4L^2}{n^2\pi^2} = \frac{4L^3}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2}$$

Parseval's theorem then implies^a

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

Note. Parseval's theorem for functions $\langle f, f \rangle = \|f\|^2$ is equivalent to Pythagoras for vectors $\langle v, v \rangle = \|v\|^2$.

 $[^]a$ Sheet 1, Q3

Remark 1. Parseval's theorem for functions is equivalent to Pythagoras' theorem for vectors in \mathbb{R}^n : we can find the norm $(\|f\|^2 = \langle f, f \rangle)$ of a linear combination by computing the sum of the norms of the components.

§1.7 Half-range series

Consider f(x) defined only on $0 \le x < L$. We can extend the range of f to be the full range $-1 \le x < L$ in two simple ways:

1. require f to be odd, so f(-x) = -f(x). Hence, $a_n = 0$ and

$$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} \, \mathrm{d}x$$

So

$$f(x) = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi x}{L}$$

which is called a Fourier sine series.

2. require f to be even, so f(-x) = f(x). In this case, $b_n = 0$ and

$$a_n = \frac{2}{L} \int_0^L f(x) \cos \frac{n\pi x}{L} \, \mathrm{d}x$$

and

$$Sof(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos \frac{n\pi x}{L}$$

which is a Fourier cosine series.

§1.8 Complex representation of Fourier series

Recall that

$$\cos \frac{n\pi x}{L} = \frac{1}{2} \left(e^{in\pi x/L} + e^{-in\pi x/L} \right);$$
$$\sin \frac{n\pi x}{L} = \frac{1}{2i} \left(e^{in\pi x/L} - e^{-in\pi x/L} \right)$$

Therefore, a Fourier series can be written as

$$f(x) = \frac{1}{2}a_0 + \frac{1}{2}\sum_{n=1}^{\infty} \left[(a_n - ib_n)e^{in\pi x/L} + (a_n + ib_n)e^{-in\pi x/L} \right]$$

$$=\sum_{m=-\infty}^{\infty}c_me^{im\pi x/L}$$

where for m>0 we have $m=n, c_m=\frac{1}{2}(a_n-ib_n)$, and for m<0 we have $n=-m, c_m=\frac{1}{2}(a_{-m}+ib_{-m})$, and where m=0 we have $c_0=\frac{1}{2}a_0$. In particular,

$$c_m = \frac{1}{2L} \int_{-L}^{L} f(x)e^{-im\pi x/L} dx$$

where the negative sign comes from the complex conjugate. This is because, for complex-valued f, g, we have

$$\langle f, g \rangle = \int_{-L}^{L} f^* g \, \mathrm{d}x$$

The orthogonality conditions are

$$\int_{-L}^{L} e^{-im\pi x/L} e^{in\pi x/L} \, \mathrm{d}x = 2L\delta_{mn}$$

Parseval's theorem now states

$$\int_{-L}^{L} f^{*}(x)f(x) dx = \int_{-L}^{L} |f(x)|^{2} dx = 2L \sum_{m=-\infty}^{\infty} |c_{m}|^{2}$$

§1.9 Self-adjoint matrices

Much of this section is a recap of IA Vectors and Matrices. Suppose that $u, v \in \mathbb{C}^N$ with inner product

$$\langle u, v \rangle = u^{\dagger} v$$

The $N \times N$ matrix A is self-adjoint, or Hermitian, if

$$\forall u, v \in \mathbb{C}^N, \langle Au, v \rangle = \langle u, Av \rangle \iff A^{\dagger} = A$$

The eigenvalues λ_n and eigenvectors v_n satisfy

$$Av_n = \lambda_n v_n$$

They have the following properties:

- 1. $\lambda_n^{\star} = \lambda_n$;
- 2. $\lambda_n \neq \lambda_m \implies \langle v_n, v_m \rangle = 0;$
- 3. we can create an orthonormal basis from the eigenvectors.

Given $b \in \mathbb{C}^n$, we can solve for x in the general matrix equation Ax = b by expressing b in terms of the eigenvector basis:

$$b = \sum_{n=1}^{N} b_n v_n$$

We seek a solution of the form

$$x = \sum_{n=1}^{N} c_n v_n$$

At this point, the b_n are known and the c_n are our target. Substituting into the matrix equation, orthogonality of basis vectors gives

$$A \sum_{n=1}^{N} c_n v_n = \sum_{n=1}^{N} b_n v_n$$
$$\sum_{n=1}^{N} c_n \lambda_n v_n = \sum_{n=1}^{N} b_n v_n$$
$$c_n \lambda_n = b_n$$
$$c_n = \frac{b_n}{\lambda_n}$$

Therefore,

$$x = \sum_{n=1}^{N} \frac{b_n}{\lambda_n} v_n$$

provided $\lambda_n \neq 0$, or equivalently, the matrix is invertible.

§1.10 Solving inhomogeneous ODEs with Fourier series

We wish to find y(x) given a source term f(x) for the general differential equation

$$\mathcal{L}y \equiv -\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = f(x)$$

with boundary conditions y(0) = y(L) = 0. The related eigenvalue problem is

$$\mathcal{L}y_n = \lambda_n y_n, \quad y_n(0) = y_n(L) = 0$$

which has solutions

$$y_n(x) = \sin \frac{n\pi x}{L}, \lambda_n = \left(\frac{n\pi}{L}\right)^2$$

We can show that this is a self-adjoint linear operator with orthogonal eigenfunctions. We seek solutions of the form of a half-range sine series. Consider

$$y(x) = \sum_{n=1}^{\infty} c_n \sin \frac{n\pi x}{L}$$

The right hand side is

$$f(x) = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi x}{L}$$

We can find b_n by

$$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} \, \mathrm{d}x$$

Substituting, we have

$$\mathcal{L}y = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \left(\sum_n c_n \sin \frac{n\pi x}{L} \right) = \sum_n c_n \left(\frac{n\pi}{L} \right)^2 \sin \frac{n\pi x}{L} = \sum_n b_n \sin \frac{n\pi x}{L}$$

By orthogonality,

$$c_n \left(\frac{n\pi}{L}\right)^2 = b_n \implies c_n = \left(\frac{L}{n\pi}\right)^2 b_n$$

Therefore the solution is

$$y(x) = \sum_{n} \left(\frac{L}{n\pi}\right)^2 b_n \sin\frac{n\pi x}{L} = \sum_{n} \frac{b_n}{\lambda_n} y_n$$

which is equivalent to the solution we found for self-adjoint matrices for which the eigenvalues and eigenvectors are known.

Example 1.8

Consider an odd square wave with L = 1, so f(x) = 1 from $0 \le x < 1$.

$$f(x) = 4\sum_{m} \frac{\sin(2m-1)\pi x}{(2m-1)\pi}$$

Then the solution to $\mathcal{L}y = f$ should be (with odd n = 2m - 1)

$$y(x) = \sum_{n} \frac{b_n}{\lambda_n} y_n = 4 \sum_{n} \frac{\sin(2m-1)\pi x}{((2m-1)\pi)^3}$$

This is exactly the Fourier series for

$$y(x) = \frac{1}{2}x(1-x)$$

so this y is the solution to the differential equation. We can in fact integrate $\mathcal{L}y=1$ directly with the boundary conditions to verify the solution. We can also differentiate the Fourier series for y twice to find the square wave.