# Part IB — Methods

Based on lectures by Dr E P Shellard and notes by thirdsgames.co.uk

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## Contents



## §1 Fourier Series

### §1.1 Periodic Functions

**Definition 1.1** (Periodic function)
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 $0 \leq x < 2L$ with period $T = 2L$. Recall that

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

**Definition 1.2** (Inner product)

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

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

[a] We will generalise this definition later when we use other eigen functions.

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

$$\begin{aligned}
\langle h_n, h_m \rangle &= \int_0^{2L} \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} \, \mathrm{d}x \\
&= \frac{1}{2} \int_0^{2L} \left( \cos \frac{(n-m)\pi x}{L} - \cos \frac{(n+m)\pi x}{L} \right) \mathrm{d}x \\
&= \frac{1}{2} \frac{L}{\pi} \left[ \frac{1}{n-m} \sin \frac{(n-m)\pi x}{L} - \frac{1}{n+m} \sin \frac{(n+m)\pi x}{L} \right]_0^{2L} \\
&= 0 \text{ when } n \neq m
\end{aligned}$$

If $n = m$, we have

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

Thus,

$$\langle h_n, h_m \rangle = \begin{cases} L\delta_{nm} & n, m \neq 0 \\ 0 & nm = 0 \end{cases} \tag{1.1}$$

Similarly, we can show

$$\langle g_n, g_m \rangle = \begin{cases} L\delta_{nm} & n, m \neq 0 \\ 0 & \text{exactly one of } m, n \text{ is zero} \\ 2L & n, m = 0 \end{cases} \tag{1.2}$$

and

$$\langle h_n, g_m \rangle = 0 \tag{1.3}$$

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

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L} \tag{1.4}$$

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

[a]Note does not require differentiability unlike a Taylor series.

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 $f$.

$$\begin{aligned}
\langle h_m, f \rangle &= \int_0^{2L} \sin\frac{m\pi x}{L} f(x)\,\mathrm{d}x \\
&= \int_0^{2L} \sin\frac{m\pi x}{L} \left( \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L} \right) \mathrm{d}x \quad \text{by substituting eq. (1.4)} \\
&= \langle h_m, b_m h_m \rangle \quad \text{by orthogonality relations eqs. (1.1) to (1.3)} \\
&= L b_m
\end{aligned}$$

Thus,

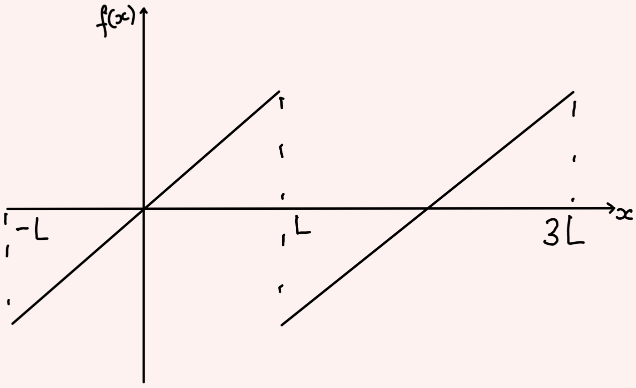
$$\begin{aligned}
b_n &= \frac{1}{L}\langle h_n, f \rangle = \frac{1}{L}\int_0^{2L} \sin\frac{n\pi x}{L} f(x)\,\mathrm{d}x \\
a_n &= \frac{1}{L}\langle g_n, f \rangle = \frac{1}{L}\int_0^{2L} \cos\frac{n\pi x}{L} f(x)\,\mathrm{d}x
\end{aligned} \tag{1.5}$$

*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.



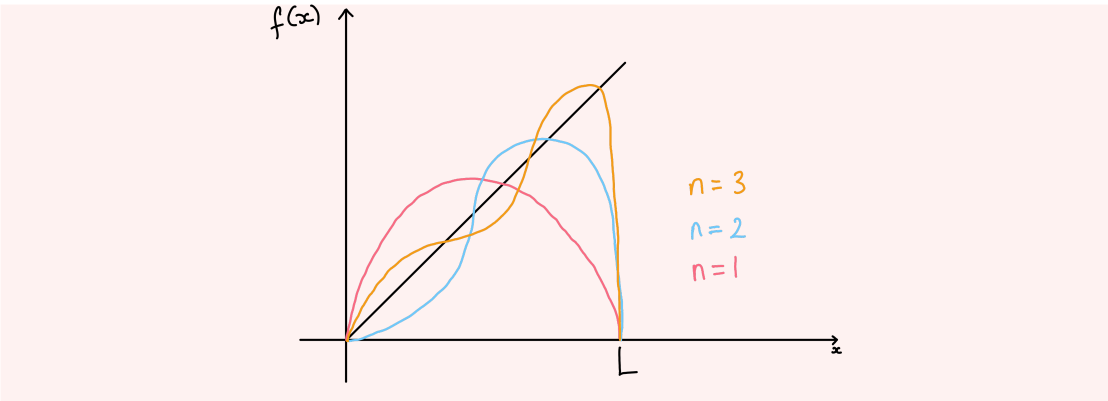

Here, $a_n = \frac{1}{L}\int_{-L}^{L} x\cos\frac{n\pi x}{L}\,\mathrm{d}x = 0$ as $x$ odd and *cos* is even.

$$
\begin{aligned}
b_n &= \frac{1}{L}\int_{-L}^{L} x\sin\frac{n\pi x}{L}\,\mathrm{d}x \\
&= \frac{2}{L}\int_{0}^{L} x\sin\frac{n\pi x}{L}\,\mathrm{d}x \ \text{ as the function we are integrating is even} \\
&= \frac{-2}{n\pi}\left[x\cos\frac{n\pi x}{L}\right]_0^L + \frac{2}{n\pi}\int_0^L \cos\frac{n\pi x}{L}\,\mathrm{d}x \\
&= \frac{-2L}{n\pi}\cos n\pi + \frac{2L}{(n\pi)^2}\sin n\pi \\
&= \frac{2L}{n\pi}(-1)^{n+1}
\end{aligned}
$$

So the sawtooth FS is

$$
\begin{aligned}
f(x) &= \frac{2L}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\sin\frac{n\pi x}{L} \qquad (1.6) \\
&= \frac{2L}{\pi}\left(\sin\frac{\pi x}{L} - \frac{1}{2}\sin\frac{2\pi x}{L} + \frac{1}{3}\sin\frac{3\pi x}{L} + \dots\right)
\end{aligned}
$$

which is slowly convergent.




*Note.* As $n \to \infty$

1. FS approx improves (convergent when cts)
2. FS $\to 0$ 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.

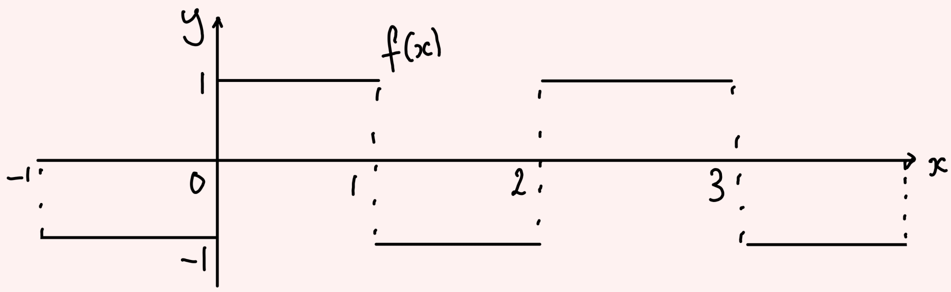
**Theorem 1.2**

If $f(x)$ has continuous derivatives up to a $p$th 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)

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




Then the Fourier series is

$$f(x) = 4 \sum_{m=1}^{\infty} \frac{\sin(2m-1)\pi x}{(2m-1)\pi} \tag{1.7}$$

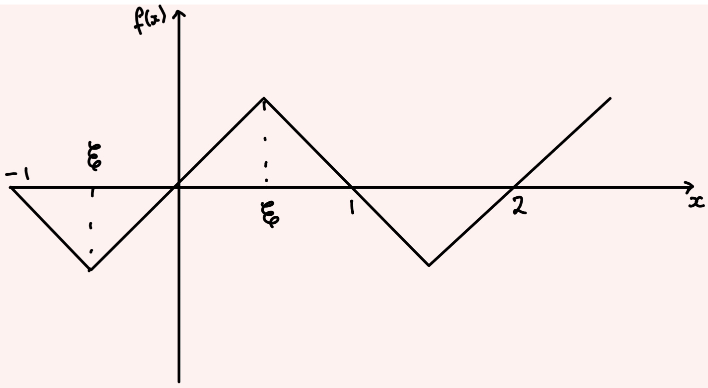
**Example 1.3** ($p = 1$)

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

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

and defined as an odd function for $-1 \leq x < 0$. The Fourier series is[a]

$$f(x) = 2 \sum_{m=1}^{\infty} \frac{\sin n\pi\xi \sin n\pi x}{(n\pi)^2} \tag{1.8}$$




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

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

[a] This is an important exercise you should do at home.

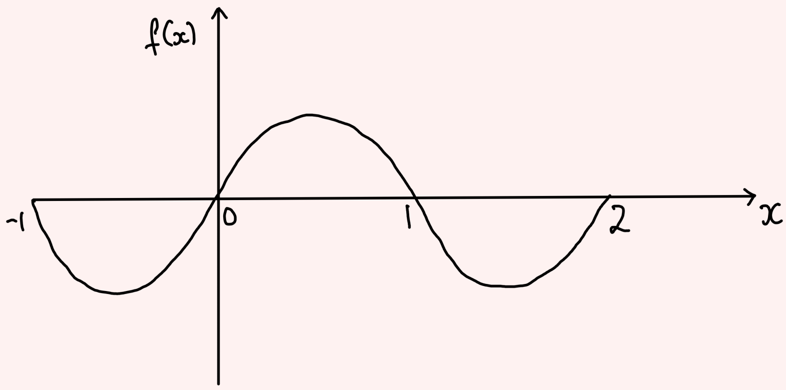
**Example 1.4** ($p = 2$)

Let

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

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

$$f(x) = 4\sum_{n=1}^{\infty}\frac{\sin(2m-1)\pi x}{((2m-1)\pi)^3} \tag{1.9}$$



**Example 1.5** ($p = 3$)

Consider[a]

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

with Fourier series

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

[a] Sheet 1, Q1

## §1.4 Integration of FS

It is always valid to take the integral of a Fourier series term by term. Defining $F(x) = \int_{-L}^{x} f(x)\,\mathrm{d}x$, 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:

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

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, eq. (1.8), 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, eq. (1.7).

## §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** (Parseval's theorem)
Suppose $f$ has Fourier coefficients $a_i, b_i$. Then

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

We can remove cross terms, since the basis functions are orthogonal. eqs. (1.1) to (1.3)

$$\begin{aligned} &= \int_0^{2L} \left[ \frac{1}{4} a_0^2 + \sum_{n=1}^{\infty} a_n^2 \cos^2 \frac{n\pi x}{L} + \sum_{n=1}^{\infty} b_n^2 \sin^2 \frac{n\pi x}{L} \right] \mathrm{d}x \\ &= L \left[ \frac{1}{2} a_0^2 + \sum_{n=1}^{\infty} (a_n^2 + b_n^2) \right] \end{aligned} \tag{1.10}$$

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 with FS eq. (1.6).

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

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]

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

[a] Sheet 1, Q3

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

## §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 $-L \le x < L$ in two simple ways:

1. require $f$ to be odd, so $f(-x) = -f(x)$. Hence, $a_n = 0$ (as cos is even) and
$$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} \, \mathrm{d}x \tag{1.11}$$
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
$$a_n = \frac{2}{L} \int_0^L f(x) \cos \frac{n\pi x}{L} \, \mathrm{d}x \tag{1.12}$$
and so
$$f(x) = \frac{1}{2} a_0 + \sum_{n=1}^{\infty} a_n \cos \frac{n\pi x}{L}$$
which is a Fourier cosine series.

## §1.8 Complex representation of Fourier series

Recall that
$$\begin{aligned} \cos \frac{n\pi x}{L} &= \frac{1}{2}\left(e^{in\pi x/L} + e^{-in\pi x/L}\right); \\ \sin \frac{n\pi x}{L} &= \frac{1}{2i}\left(e^{in\pi x/L} - e^{-in\pi x/L}\right) \end{aligned}$$
Therefore, a Fourier series can be written as
$$\begin{aligned} f(x) &= \frac{1}{2} a_0 + \frac{1}{2} \sum_{n=1}^{\infty} \left[(a_n - ib_n) e^{in\pi x/L} + (a_n + ib_n) e^{-in\pi x/L}\right] \\ &= \sum_{m=-\infty}^{\infty} c_m e^{im\pi x/L} \end{aligned} \tag{1.13}$$
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,
$$c_m = \frac{1}{2L} \int_{-L}^{L} f(x) e^{-im\pi x/L} \, \mathrm{d}x \tag{1.14}$$
where the negative sign comes from the complex conjugate. This is because, for complex-valued $f, g$, we have

**Definition 1.4** (Complex inner product)

$$\langle f, g\rangle = \int_{-L}^{L} f^{\star\,[a]} g \,\mathrm{d}x$$

[a] $f^\star$ is the complex conjugate of $f$.

The orthogonality conditions are

$$\int_{-L}^{L} e^{-im\pi x/L} e^{in\pi x/L} \,\mathrm{d}x = 2L\delta_{mn} \tag{1.15}$$

Parseval's theorem now states

$$\int_{-L}^{L} f^\star(x) f(x) \,\mathrm{d}x = \int_{-L}^{L} |f(x)|^2 \,\mathrm{d}x = 2L \sum_{m=-\infty}^{\infty} |c_m|^2$$

## §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

$$\langle u, v\rangle = u^\dagger v \tag{1.16}$$

**Definition 1.5** (Hermitian matrix)

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 $\lambda_n$ and eigenvectors $v_n$ satisfy

$$Av_n = \lambda_n v_n \tag{1.17}$$

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

$$Ax = b \tag{1.18}$$

Express $b$ 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 eq. (1.18), orthogonality of basis vectors gives

$$\begin{aligned} A\sum_{n=1}^{N} c_n v_n &= \sum_{n=1}^{N} b_n v_n \\ \sum_{n=1}^{N} c_n \lambda_n v_n &= \sum_{n=1}^{N} b_n v_n \end{aligned}$$

As the eigenvector basis is orthogonal we can equate coefficients

$$\begin{aligned} c_n \lambda_n &= b_n \\ c_n &= \frac{b_n}{\lambda_n} \end{aligned}$$

Therefore,

$$x = \sum_{n=1}^{N} \frac{b_n}{\lambda_n} v_n \tag{1.19}$$

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 driving/ source term $f(x)$ for the general differential equation

$$\mathcal{L}y \equiv -\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} = f(x) \tag{1.20}$$

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

$$y_n(x) = \sin\frac{n\pi x}{L}, \;\; \lambda_n = \left(\frac{n\pi}{L}\right)^2 \tag{1.21}$$

We can show that this is a self-adjoint linear operator[1] 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 into eq. (1.20), we have

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

$$\text{So } \sum_n c_n \left(\frac{n\pi}{L}\right)^2 \sin \frac{n\pi x}{L} = \sum_n b_n \sin \frac{n\pi x}{L}$$

By orthogonality eq. (1.1),

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

Therefore the solution is

$$y(x) = \sum_n \left(\frac{L}{n\pi}\right)^2 b_n \sin \frac{n\pi x}{L} = \sum_n \frac{b_n}{\lambda_n} y_n \tag{1.22}$$

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

**Example 1.8** (Odd square wave)

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

$$f(x) = 4 \sum_m \frac{\sin(2m-1)\pi x}{(2m-1)\pi} \text{ by eq. (1.7)}$$

Then the solution to $\mathcal{L}y = f$ eq. (1.22) should be (with odd $n = 2m - 1$)

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

[1] https://math.stackexchange.com/questions/4356100/why-is-the-second-derivative-operator-self-adjoint

This is exactly the Fourier series for

$$y(x) = \frac{1}{2}x(1-x) \text{ by eq. (1.9)}$$

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.