IB Methods

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Contents

Part I

Self-Adjoint ODE'S

1 Fourier Series

1.1 Periodic Functions

A function $f(x)$ is **periodic** if

$$f(x+T) = f(x),$$

where T is the period.

Example 1.1. Consider simple harmonic motion. We have

$$y = A\sin\omega t,$$

where A is the amplitude and the period $T = 2\pi/\omega$, with angular frequency ω.

Consider the set of functions

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

which are periodic on the interval $0 \leq x < 2L$. Recall the identities

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

Define the **inner product** for two periodic functions f, g on the interval $[0, 2L)$

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

I claim that the functions g_n, h_m are **mutually orthogonal**. Indeed,

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

This works for $n \neq m$. For $n = m$,

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

Hence, we can put these together to get

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

Similarly, we can show

$$\langle g_n, g_m \rangle = \begin{cases} L\delta_{nm}, & \forall n, m \neq 0, \\ 2L\delta_{0n}, & m = 0. \end{cases} \quad \text{and} \quad \langle h_n, g_m \rangle = 0.$$

1.2 Definition of Fourier series

We can express any 'well-behaved' periodic function $f(x)$ with period $2L$ as

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

where a_n, b_n are constant such that the right hand side is convergent for all x where f is continuous. At a discontinuity x, the Fourier series approaches the midpoint

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

1.2.1 Fourier Coefficients

Consider the inner product

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

by the orthogonality relations. Hence we find that

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

Remark.

(i) a_n includes $n = 0$, since $\frac{1}{2}a_0$ is the **average**

$$\langle f(x) \rangle = \frac{1}{2L} \int_0^{2L} f(x) \, \mathrm{d}x.$$

(ii) The range of integration is over one period, so we may take the integral over $[0, 2L)$ or $[-L, L)$.

(iii) We can think of the Fourier series as a decomposition into harmonics. The simplest Fourier series are the sine and cosine functions.

Example 1.2 (Sawtooth wave)**.**

Consider the function $f(x) = x$ for $-L \leq x < L$, periodic with period $T = 2L$. The cosine coefficients are

$$a_n = \frac{1}{L} \int_{-L}^{L} x \cos \frac{n\pi x}{L} \, \mathrm{d}x = 0,$$

as $x \cos \omega x$ is odd. The sine coefficients are

$$\begin{aligned} b_n &= \frac{2}{L} \int_0^L x \sin \frac{n\pi x}{L} \, \mathrm{d}x \\ &= -\frac{2}{n\pi} \left[x \cos \frac{n\pi x}{L} \right]_0^L + \frac{2}{n\pi} \int_0^L \cos \frac{n\pi x}{L} \, \mathrm{d}x \\ &= -\frac{2L}{n\pi} \cos n\pi + \frac{2L}{(n\pi)^2} \sin n\pi = \frac{2L}{n\pi} (-1)^{n+1}. \end{aligned}$$

So the sawtooth Fourier series is

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

With Fourier series, we can construct functions with only finitely many discontinuities, the topologist's sine curve, and the Weierstrass function.

1.3 The Dirichlet Conditions (Fourier's theorem)

These are sufficiency conditions for a "well-behaved" function to have a unique Fourier series:

Proposition 1.1. *If $f(x)$ is a bounded periodic function (period $2L$) with a finite number of minima, maxima and discontinuities in $0 \leq x < 2L$, then the Fourier series converges to $f(x)$ at all points where f is continuous; at discontinuities the series converges to the midpoint.*

Remark.

(i) These are weak conditions (in contrast to Taylor series), but pathological functions are excluded, such as

$$f(x) = \frac{1}{x}, \quad f(x) = \sin\frac{1}{x}, \quad f(x) = \begin{cases} 0 & x \in \mathbb{Q}, \\ 1 & x \notin \mathbb{Q}. \end{cases}$$

(ii) The converse is not true.

(iii) The proof is difficult.

1.3.1 Convergence of Fourier Series

Theorem 1.1. *If $f(x)$ has continuous derivatives up to the p'th derivative, which is discontinuous, then the Fourier series converges as $\mathcal{O}(n^{-(p+1)})$.*

Example 1.3. Take the square wave, with $p = 0$.

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

The Fourier series is

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

We now look at the general "see-saw" wave, with $p = 1$. Here

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

and odd for $-1 \leq x < 0$. The Fourier series is

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

For $\xi = 1/2$, we have

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

For $p = 2$, take $f(x) = x(1-x)/2$ on $0 \leq x < 1$, and odd for $-1 \leq x < 0$. The Fourier series is

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

Consider $f(x) = (1-x^2)^2$, for $p = 3$. Then $a_n = \mathcal{O}(n^{-4})$.

1.3.2 Integration of Fourier Series

It is always valid to integrate the Fourier series of $f(x)$ term-by-term to obtain

$$F(x) = \int_{-L}^{x} f(x)\,\mathrm{d}x,$$

because $F(x)$ satisfies the Dirichlet conditions if $f(x)$ does.

1.3.3 Differentiation of Fourier Series

Differentiation needs to be done with great care. Consider the square wave. We differentiate it to get

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

But this is unbounded.

Theorem 1.2. *If $f(x)$ is continuous and satisfies the Dirichlet conditions, and $f'(x)$ satisfies the Dirichlet conditions, then $f'(x)$ can be found by term-by-term differentiation of the Fourier series of $f(x)$.*

Example 1.4. If we differentiate the see-saw with $\xi = 1/2$, then we get an offset square wave.

1.4 Parseval's Theorem

This gives the relation between the integral of the square of a function and the sum of the squares of the Fourier coefficients:

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

This is also called the **completeness relation** because the left hand side is always greater than equal to the right hand side if any basis is missing.

Example 1.5. Take the sawtooth wave. We have

$$LHS = \int_{-L}^{L} x^2 \,\mathrm{d}x = \frac{2}{3}L^3,$$

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

Therefore, we obtain
$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

1.5 Alternative Fourier Series

1.5.1 Half-range Series

Consider $f(x)$ defined only on $0 \leq x < L$. Then we can extend its range over $-L \leq x < L$ in two simple ways:

(i) Require it to be odd, so $f(-x) = -f(x)$. Then $a_n = 0$, and
$$b_n = \frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} \, \mathrm{d}x.$$
This is a Fourier sine series.

(ii) Require it to be even, so $f(-x) = f(x)$. Then $b_n = 0$,
$$a_n = \frac{2}{L} \int_0^L f(x) \cos \frac{n\pi x}{L} \, \mathrm{d}x.$$
This is a Fourier cosine series.

1.5.2 Complex Representation

Recall that
$$\cos \frac{n\pi x}{L} = \frac{1}{2}\left(e^{in\pi x/L} + e^{-in\pi x/L}\right), \quad \sin \frac{n\pi x}{L} = \frac{1}{2i}\left(e^{in\pi x/L} - e^{-in\pi x/L}\right).$$
So our Fourier series becomes
$$\begin{aligned} f(x) &= \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos \frac{n\pi x}{L} + \sum_{n=1}^{\infty} b_n \sin \frac{n\pi x}{L} \\ &= \frac{1}{2}a_0 + \frac{1}{2}\sum_{n=1}^{\infty}(a_n - ib_n)e^{in\pi x/L} + \frac{1}{2}\sum_{n=1}^{\infty}(a_n + ib_n)e^{-in\pi x/L} \\ &= \sum_{m=-\infty}^{\infty} c_m e^{im\pi x/L}. \end{aligned}$$

The coefficients c_m satisfy

$$c_m = \begin{cases} \frac{1}{2}(a_m - ib_m) & m > 0, \\ \frac{1}{2}a_0 & m = 0, \\ \frac{1}{2}(a_{-m} + ib_{-m}) & m < 0. \end{cases}$$

Equivalently,

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

Our inner product in the complex representation is

$$\langle f, g \rangle = \int f^* g \, \mathrm{d}x.$$

This is orthogonal, as

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

and satisfies Parseval's theorem as a result:

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

1.6 Fourier Series Motivations

1.6.1 Self-adjoint matrices

Suppose $\mathbf{u}, \mathbf{v}$ are complex N-vectors with inner product $\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^\dagger \mathbf{v}$. Then matrix A is self-adjoint (or Hermitian) if

$$\langle A\mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{u}, A\mathbf{v} \rangle \implies A^\dagger = A.$$

The eigenvalues $\lambda_1, \ldots, \lambda_N$ of A satisfy the following properties:

(i) The eigenvalues are real: $\lambda_n^* = \lambda_n$.

(ii) If $\lambda_n \neq \lambda_m$, then their respective eigenvectors are orthogonal: $\langle \mathbf{v}_n, \mathbf{v}_m \rangle = 0$.

(iii) If we rescale our eigenvectors then $\{\mathbf{v}_1, \ldots, \mathbf{v}_N\}$ form an orthonormal basis.

Given $\mathbf{b}$, we can try to solve for $\mathbf{x}$ in $A\mathbf{x} = \mathbf{b}$. Express

$$\mathbf{b} = \sum_{n=1}^{N} b_n \mathbf{v}_n, \quad \mathbf{x} = \sum_{n=1}^{N} c_n \mathbf{v}_n.$$

Substituting into the equation,

$$
\begin{aligned}
A\mathbf{x} &= \sum_{n=1}^{N} A c_n \mathbf{v}_n = \sum_{n=1}^{N} c_n \lambda_n \mathbf{v}_n, \\
\mathbf{b} &= \sum_{n=1}^{N} b_n \mathbf{v}_n.
\end{aligned}
$$

Equating and using orthogonality,

$$c_n \lambda_n = b_n \implies c_n = \frac{b_n}{\lambda_n}.$$

Hence the solution is

$$\mathbf{x} = \sum_{n=1}^{N} \frac{b_n}{\lambda_n} \mathbf{v}_n.$$

1.6.2 Solving inhomogeneous ODE with Fourier series

Take the following problem: We wish to find $y(x)$ given $f(x)$ for which

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

subject to the boundary conditions $y(0) = y(L) = 0$. The related eigenvalue problem is

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

This has eigenfunctions and eigenvalues

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

Note that $\mathcal{L}$ is a self-adjoint ODE with orthogonal eigenfunctions. Thus we seek solutions as a half-range sine series. We try

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

and expand

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

Substituting this in,

$$\begin{aligned}\mathcal{L}y &= -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\sum_n c_n \sin\frac{n\pi x}{L}\right) = \sum_{n=1}^{\infty} c_n \left(\frac{n\pi}{L}\right)^2 \sin\frac{n\pi x}{L} \\ &= \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L}.\end{aligned}$$

By orthogonality, we have

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

Thus the solution is

$$y(x) = \sum_{n=1}^{\infty}\left(\frac{L}{n\pi}\right)^2 b_n \sin\frac{n\pi x}{L} = \sum_{n=1}^{\infty}\frac{b_n}{\lambda_n} y_n.$$

This is similar to a self-adjoint matrix.

Example 1.6. Consider the square wave on $L = 1$, as an odd function. This has Fourier series

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

So the solution should be

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

This is the Fourier series for $y(x) = x(1-x)/2$.

2 Sturm-Liouville theory

2.1 Second-order linear ODEs

We wish to solve a general inhomogeneous ODE

$$\mathcal{L}y = \alpha(x)y'' + \beta(x)y' + \gamma(x)y = f(x).$$

- The **homogeneous** equation $\mathcal{L}y = 0$ has two independent solutions $y_1(x)$, $y_2(x)$. The **complementary function** $y_c(x)$ is the general solution of

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

  where A, B are constants.

- The **inhomogeneous** equation $\mathcal{L}y = f(x)$ has a special solution, the **particular integral** $y_p(x)$. The general solution is then

  $$y(x) = y_p(x) + Ay_1(x) + By_2(x).$$

- Two **boundary** or **initial** conditions are required to determine A, B:

  (a) **Boundary conditions** require us to solve the equation on $a < x < b$ given y at $x = a, b$ (Dirichlet conditions), or given y' at $x = a, b$ (Neumann conditions), or given a mixed value $y + ky'$. Boundary conditions are often assumed to be $y(a) = y(b)$, to admit the trivial solution $y \equiv 0$. This can be done by adding complementary functions

  $$\tilde{y} = y + A_1y_1 + By_2.$$

  (b) **Initial condition** require us to solve the equation for $x \geq a$, given y and y' at $x = a$.

2.1.1 General eigenvalue problem

To solve the equation employing eigenfunction expansion, we are required to solve the related eigenvalue problem

$$\alpha(x)y'' + \beta(x)y' + \gamma(x)y = -\lambda\rho(x)y,$$

with specified boundary conditions. This forms often occurs in higher dimensions, after separation of variables.

2.2 Self-adjoint operators

For two complex-valued functions f, g on $a \leq x \leq b$, we can define the **inner product**

$$\langle f, g\rangle = \int_a^b f^*(x)g(x)\,\mathrm{d}x.$$

The norm is then $\|f\| = \langle f, f\rangle^{1/2}$.

2.2.1 Sturm-Liouville equation

The eigenvalue problem greatly simplifies if $\mathcal{L}$ is **self-adjoint**, that is, it can be expressed in **Sturm-Liouville form**

$$\mathcal{L}y \equiv -(\rho y')' + qy = \lambda\omega y,$$

where the **weight function** $\omega(x)$ is non-negative. We can convert to Sturm-Liouville form by multiplying by an integrating factor $F(x)$ to find

$$F\alpha y'' + F\beta y' + F\gamma y = -\lambda F\rho y.$$

This gives

$$\frac{\mathrm{d}}{\mathrm{d}x}(F\alpha y') - F'\alpha y' - F\alpha' y' + F\beta y' + F\gamma y = -\lambda F\rho y.$$

Eliminating y' terms, we require

$$F'\alpha = F(\beta - \alpha') \implies \frac{F'}{F} = \frac{\beta - \alpha'}{\alpha}.$$

Solving, we get

$$F(x) = \exp\left(\int^x \frac{(\beta - \alpha')}{\alpha}\,\mathrm{d}x\right),$$

and $(F\alpha y')' + F\gamma y = -\lambda F\rho y$. So $\rho(x) = F(x)\alpha(x)$, $q(x) = -F(x)\gamma(x)$, and $\omega(x) = F(x)\rho(x)$. This is non-negative as $F(x) > 0$.

Example 2.1. Take the Hermite equation

$$y'' - 2xy' + 2ny = 0.$$

Putting this into Sturm-Liouville form, we have $\alpha = 1$, $\beta - 2x$, $\gamma = 0$ and $\lambda\rho = 2n$. Thus we take

$$F = \exp\left(\int^x \frac{-2x}{2}\,\mathrm{d}x\right) = e^{-x^2}.$$

Hence

$$\mathcal{L}y \equiv -(e^{-x^2}y')' = 2ne^{-x^2}y.$$

2.2.2 Self-adjoint definition

A linear operator $\mathcal{L}$ is **self-adjoint** on $a \leq x \leq b$ for all pairs of functions y_1, y_2 satisfying boundary conditions, if

$$\langle y_1, \mathcal{L}y_2 \rangle = \langle \mathcal{L}y_1, y_2 \rangle,$$

or

$$\int_a^b y_1^*(x)\mathcal{L}y_2(x)\,\mathrm{d}x = \int_a^b (\mathcal{L}y_1(x))^* y_2(x)\,\mathrm{d}x.$$

Substituting the Sturm-Liouville form into this equation gives

$$\begin{aligned}
\langle y_1, \mathcal{L}y_2 \rangle - \langle \mathcal{L}y_1, y_2 \rangle &= \int_a^b [-y_1(\rho y_2')' + y_1 q y_2 + y_2(\rho y_1')' - y_2 q y_1]\,\mathrm{d}x \\
&= \int_a^b [-(\rho y_1 y_2')' + (\rho y_1' y_2)']\,\mathrm{d}x \\
&= [-\rho y_1 y_2' + \rho y_1' y_2]_a^b = 0.
\end{aligned}$$

for given boundary conditions at $x = a, b$. Suitable boundary conditions include:

- $y(a) = y(b) = 0$, $y'(a) = y'(b) = 0$, or mixed boundary condition $y + ky' = 0$;
- Periodic functions $y(a) = y(b)$;
- Singular points of the ODE $\rho(a) = \rho(b) = 0$;
- Combinations of the above.

2.3 Properties of self-adjoint operators

Self-adjoint operators satisfy many similar properties to self-adjoint matrices:

1. The eigenvalues λ_n are real.
2. The eigenfunctions y_n are orthogonal.
3. The eigenfunctions y_n form a complete set.

Index