

Solutions of differential equations.

We will consider a special class of differential eqns, that are called Sturm-Liouville problem

$$\frac{d}{dx} \left(f(x) \frac{dy}{dx} \right) - g(x)y + \lambda w(x)y = 0$$

Such equations often appear in various physics problems, for example in solutions of Schrödinger equation:

$$\hat{H}\psi(x) = E\psi(x)$$

One has to solve this equation for a particular problem (i.e. for different forms of $\hat{H} = \hat{K} + \hat{V}$), find all real eigenvalues E_n of energy, and the corresponding eigenfunctions ψ_n .

We also usually search for a solution at a specific region $a \leq x \leq b$, and our solution must obey some imposed boundary conditions, for example:

Dirichlet conditions: $y(a) = y(b) = 0$

Neumann conditions: $y'(a) = y'(b) = 0$

Let's show that solutions $\{\psi_n\}$ of the Sturm-Liouville problem corresponding to different eigenvalues λ_n are orthogonal.

But first we need to define the product of two functions:

$$\langle u(x) | v(x) \rangle = \int_a^b u^*(x) v(x) \cdot w(x) dx$$

$w(x)$ is a weight function

(It will determine the asymptotic behavior of all solutions)

So let's check that $\langle y_n | y_m \rangle = 0$ if $\lambda_n \neq \lambda_m$

(and we will assume all $\{y_n\}$ are real?)

$$y_m \times \frac{d}{dx} \left(f(x) \frac{dy_n}{dx} \right) - g(x) y_m + \lambda_n w(x) y_n(x) = 0$$

$$y_n \times \frac{d}{dx} \left(f(x) \frac{dy_m}{dx} \right) - g(x) y_n + \lambda_m w(x) y_m(x) = 0$$

$$\int_a^b \left[y_m \frac{d}{dx} \left(f(x) \frac{dy_n}{dx} \right) - y_n \frac{d}{dx} \left(f(x) \frac{dy_m}{dx} \right) \right] dx + (\lambda_n - \lambda_m) \int_a^b w(x) y_n(x) y_m(x) dx = 0$$

$$= \left[\left(y_m f(x) \frac{dy_n}{dx} \right) \Big|_a^b - \left(y_n f(x) \frac{dy_m}{dx} \right) \Big|_a^b \right] - \int_a^b \left(f(x) \frac{dy_n}{dx} \frac{dy_m}{dx} - f(x) \frac{dy_m}{dx} \frac{dy_n}{dx} \right) dx = 0$$

≈ 0 because of the boundary conditions

Thus $(\lambda_n - \lambda_m) \int_a^b w(x) y_n(x) y_m(x) dx = 0$, and if $\lambda_n \neq \lambda_m$ solutions $y_n(x)$ and $y_m(x)$ are orthogonal $\langle y_n | y_m \rangle = 0$

It is also possible to show that solutions $\{y_n\}$ form a complete set of functions, i.e. any function $F(x)$ can be decomposed into a sum of $\{y_n\}$

$$F(x) = \sum_{n=0}^{\infty} a_n y_n(x)$$

Using the orthogonality :

$$\int_a^b F(x) y_k(x) w(x) dx = \sum_{n=0}^{\infty} a_n \int_a^b y_n(x) y_k(x) w(x) dx = a_k \int_a^b y_k^2 w(x) dx$$

$$a_k = \frac{\int_a^b F(x) y_k(x) w(x) dx}{\int_a^b y_k^2 w(x) dx}$$

Fourier series is an example of Sturm-Liouville problem

$$\frac{d^2}{dx^2} y + k^2 y = 0 \Rightarrow w(x) = 1, f(x) = 1, g(x) = 0, \lambda = k^2$$

With Dirichlet boundary conditions

$$y(L) = y(-L) = 0 \quad y_n = \sin \frac{\pi n x}{L}, k_n = \frac{\pi n}{L}$$

With Neumann boundary conditions

$$y'(L) = y'(-L) = 0 \quad y_n = \cos \frac{\pi n x}{L}, k_n = \frac{\pi n}{L}$$

Another important example: Legendre polynomials

$$\frac{d}{dx} \left[(1-x^2) \frac{dy}{dx} \right] + l(l+1)y = 0 \quad \text{or} \quad (1-x^2)y'' - 2x y' + l(l+1)y = 0$$

We will search for solutions in forms of power series that are finite at the interval $-1 \leq x \leq 1$

$$y(x) = \sum_{n=0}^{\infty} a_n x^n = a_0 + a_1 x + a_2 x^2 + \dots$$

$$y'(x) = \sum_{n=1}^{\infty} a_n \cdot n x^{n-1} = a_1 + 2a_2 x + 3a_3 x^2 + \dots$$

$$y''(x) = \sum_{n=2}^{\infty} a_n n(n-1) x^{n-2} = 2a_2 + 6a_3 x + \dots$$

Substitute y, y' and y'' into the Legendre eqn

$$(1-x^2)(2a_2 + 6a_3 x + \dots) - 2x(a_1 + 2a_2 x + 3a_3 x^2) + l(l+1)(a_0 + a_1 x + a_2 x^2 + \dots) = 0$$

and then collect the coefficient for each power of x and make sure each of them is zero.

$$x^0: 2a_2 + l(l+1)a_0 = 0$$

$$a_2 = -\frac{l(l+1)}{2} a_0$$

$$x^1: 6a_3 - 2a_1 + l(l+1)a_1 = 0$$

$$a_3 = \frac{l^2 l^2 - 2}{6} a_1 = \frac{(l+2)(l-1)}{6} a_1$$

For an arbitrary x^n

$$(1-x^2) \sum_{n=2}^{\infty} a_n n(n-1)x^{n-2} - 2x \sum_{n=1}^{\infty} a_n \cdot nx^{n-1} + l(l+1) \sum_{n=0}^{\infty} a_n x^n = 0$$

$$\sum_{n=2}^{\infty} a_n n(n-1)x^{n-2} - \sum_{n=2}^{\infty} a_n n(n-1)x^n - 2 \sum_{n=1}^{\infty} a_n nx^n + l(l+1) \sum_{n=0}^{\infty} a_n x^n = 0$$

$\downarrow n \rightarrow n+2$

$$\sum a_{n+2} (n+2)(n+1)x^n - \dots$$

$$a_{n+2} (n+2)(n+1) - a_n n(n-1) - 2a_n \cdot n + l(l+1) a_n = 0$$

$$a_{n+2} = \frac{[n(n+1) - l(l+1)]}{(n+1)(n+2)} a_n = - \frac{(l+n+1)(l-n)}{(n+1)(n+2)} a_n =$$

$$= \frac{(l+n-1)(l-n)}{(n+1)(n+2)} \frac{(l+n-3)(l-n+2)}{n(n-1)} a_{n-2} = \dots$$

Thus the general solution of the Legendre eqn is

$$y = a_0 \left(1 - \frac{l(l+1)}{2} x^2 + \frac{(l+3)(l+1)l(l-2)}{4 \cdot 3 \cdot 2 \cdot 1 \cdot 4!} x^4 - \dots \right) +$$

$$+ a_1 \left(x - \frac{(l+2)(l+1)}{3!} x^3 + \frac{(l+4)(l+2)(l-1)(l-3)}{5!} x^5 - \dots \right)$$

This infinite series converges for $|x| < 1$.

A special case is $l = \text{integer number}$

Then one series will become a finite polynomial, and the other will still be an infinite series diverging at $x = \pm 1$.

Thus to have a solution for $|x| \leq 1$, we have to keep the polynomial solution, and set the other series to zero.

These are Legendre polynomials

Traditional normalization of Legendre polynomials

$$P_0(1) = 1$$

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$\ell=2 : P_2 = a_0 \left(1 - \frac{2 \cdot 3}{2} x^2\right) \Rightarrow -2a_0 = 1 \quad a_0 = -\frac{1}{2}$$

$$P_2(x) = \frac{1}{2} (3x^2 - 1)$$

Legendre polynomials are eigenfunction of the parity operator

$$P_\ell(x) = P_\ell(-x) \text{ for even } \ell, \text{ and } P_\ell(x) = -P_\ell(-x) \text{ for odd } \ell$$

$$P_\ell(x) = (-1)^\ell P_\ell(-x)$$

Rodriges formula to derive Legendre polynomials

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} (x^2 - 1)^\ell$$

Before proving this, let's first notice that if $V(x) = (x^2 - 1)^\ell$

$$(x^2 - 1) \frac{dV}{dx} = (x^2 - 1) 2\ell x (x^2 - 1)^{\ell-1} = 2\ell x \cdot V(x)$$

We will also use the Leibniz's differentiation rule:

$$\frac{d^n}{dx^n} (f(x) \cdot g(x)) = \frac{d^{n-1}}{dx^{n-1}} (f(x)g'(x) + g(x)f'(x)) = \frac{d^{n-2}}{dx^{n-2}} (fg'' + 2f'g' + f''g) =$$

$$= \sum_{k=0}^n \binom{n}{k} f^{(k)}(x) g^{(n-k)}(x)$$

That means that

$$\frac{d^{\ell+1}}{dx^{\ell+1}} \left[(x^2 - 1) \frac{dV}{dx} \right] = (x^2 - 1) \frac{d^{\ell+2}}{dx^{\ell+2}} V + 2x(\ell+1) \frac{d^{\ell+1}}{dx^{\ell+1}} V + \frac{\ell(\ell+1)}{2} \cdot 2 \frac{d^\ell}{dx^\ell} V$$

on the other hand //

$$\frac{d^{\ell+1}}{dx^{\ell+1}} (2\ell x \cdot V) = 2\ell x \frac{d^{\ell+1}}{dx^{\ell+1}} V + 2\ell(\ell+1) \frac{d^\ell}{dx^\ell} V$$

$$(x^2 - 1) \frac{d^2}{dx^2} \left(\frac{d^\ell}{dx^\ell} \cdot V \right) + 2x \frac{d}{dx} \left(\frac{d^\ell}{dx^\ell} V \right) - \ell(\ell+1) \frac{d^\ell}{dx^\ell} V = 0$$

$$(1-x^2) \frac{d^2}{dx^2} V^{(\ell)} - 2x \frac{d}{dx} V^{(\ell)} + \ell(\ell+1) V^{(\ell)} = 0$$

Thus $y = A \cdot v^l$ is a solution of Legendre eqn.

To make it the Legendre polynomials one needs to take care of normalization

$$P_l(1) = 1 = A \cdot \frac{d^l}{dx^l} (x^2 - 1)^l \Big|_{x=1} = A \cdot \frac{d^l}{dx^l} (x-1)^l (x+1)^l \Big|_{x=1} =$$

Any terms with $(x-1)$ will be zero at $x=1$.

So the only non-zero term is when $(x-1)^l$ is differentiated l times, and $(x+1)^l$ term is left as is.

$$= A \cdot l! (x+1)^l \Big|_{x=1} = A \cdot l! \cdot 2^l \Rightarrow A = \frac{1}{2^l l!}$$

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2 - 1)^l$$