Lecture 17

Last time we proved that Legendre polynomials are a complete, orthogonal set

$$\int_{-1}^{1} P_\ell(x) P_m(x)\,dx = \frac{2}{2\ell+1}\delta_{\ell m}$$

- then we can expand any function on $[-1,1]$ in terms of Legendre polynomials as

$$f(x) = \sum_{\ell=0}^{\infty} c_\ell P_\ell(x)$$

just like we do for Fourier series.

<u>Example:</u> Expand the following function as a Legendre series:

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

②

So we need to find the coefficients $\{c_\ell\}_\ell$

By calcuting the following, we can get them:

$$\int_{-1}^{1} f(x)\, P_m(x)\, dx$$

$$= \sum_{\ell=0}^{\infty} c_\ell \int_{-1}^{1} P_\ell(x)\, P_m(x)\, dx$$

$$= \sum_{\ell=0}^{\infty} c_\ell\, \delta_{\ell,m} \frac{2}{2\ell+1}$$

$$= c_m \frac{2}{2m+1}$$

then we find that

to get c_0: $\int_{-1}^{1} f(x) P_0(x) = c_0 \cdot 2$

$$= \int_0^1 dx = 1 \Rightarrow c_0 = \frac{1}{2}$$

to get c_1:

$$\int_{-1}^{1} f(x)\, P_1(x)\, dx = c_1 \cdot \frac{2}{3}$$

$$= \int_0^1 x\, dx = \frac{1}{2}$$

$$\Rightarrow \quad c_1 = \frac{3}{4}$$

to get c_2:

$$\int_{-1}^{1} f(x)\, P_2(x)\, dx = c_2 \cdot \frac{2}{5}$$

$$= \int_0^1 \left[\frac{3}{2}x^2 - \frac{1}{2}\right] dx$$

$$= \frac{1}{2} - \frac{1}{2} = 0 .$$

continuing, we get that

$$f(x) = \frac{1}{2} P_0(x) + \frac{3}{4} P_1(x)$$

$$- \frac{7}{16} P_3(x) + \frac{11}{32} P_5(x) + \ldots$$

Interestingly, the Legendre series gives the best polynomial least-squares fit to a function defined on the interval $[-1, 1]$

- That is, suppose the goal is to approximate $f(x)$ on $[-1,1]$ w/ an nth degree polynomial:

$$Q_n(x) = \sum_{j=0}^{n} a_j x^j$$

- How to measure the quality of the approximation? Can use the least-squares criterion:

$$\int_{-1}^{1} [f(x) - Q_n(x)]^2 \, dx$$

Alternatively, there are coefficients $\{b_\ell\}_\ell$

such that

$$Q_n(x) = \sum_{\ell=0}^{n} b_\ell P_\ell(x)$$

where these are the normalized Legendre polynomials

How to choose $\{b_\ell\}_\ell$ to minimize the error?

Pick them to be Legendre coefficients! $c_\ell = \int_{-1}^{1} f(x) P_\ell(x)\,dx$

How to see this?

Consider that error is equal to

$$\int_{-1}^{1} \left[f(x) - \sum_{\ell=0}^{n} b_\ell P_\ell(x)\right]^2 dx$$

$$= \int_{-1}^{1} \left([f(x)]^2 - 2\sum_{\ell=0}^{n} b_\ell f(x) P_\ell(x) + \sum_{\ell=0,\ell'=0}^{n} b_\ell b_{\ell'} P_\ell(x) P_{\ell'}(x) \right) dx$$

⑥

$$= \int_{-1}^{1} [f(x)]^2 dx - 2\sum_{l=0}^{n} b_l \int_{-1}^{1} f(x) P_l(x) dx$$

$$+ \sum_{l=0, l'=0}^{n} b_l b_{l'} \int_{-1}^{1} P_l(x) P_{l'}(x) dx$$

$$= \int_{-1}^{1} [f(x)]^2 dx - 2\sum_{l=0}^{n} b_l c_l$$

$$+ \sum_{l=0, l'=0}^{n} b_l b_{l'} \delta_{l,l'}$$

$$= \quad '' \quad - \quad '' \quad + \sum_{l=0}^{n} b_l^2$$

$$= \int_{-1}^{1} [f(x)]^2 dx + \sum_{l=0}^{n} b_l^2 - 2 b_l c_l$$

$$= \int_{-1}^{1} \{f(x)]^2 dx + \sum_{l=0}^{n} (b_l - c_l)^2 - c_l^2$$

$\therefore$ clear that we then minimize error by setting $b_l = c_l$.

Associated Legendre functions

When solving the Schrödinger equation for hydrogen

$$\frac{\hbar^2}{2m} \nabla^2 \psi + \underbrace{\frac{e^2}{r}}_{} \psi = E\psi$$

Coulomb potential for proton + electron

or $\nabla^2 \psi + \frac{1}{\rho} \psi = \varepsilon \psi$ in dimensionless form

guess a solution for which the variables are separable:

$$\psi(\rho, \theta, \phi) = R(\rho) \underbrace{\Theta(\theta) \Phi(\varphi)}_{Y(\theta, \varphi)}$$

where

$$Y(\theta, \varphi) = y_{l,m}(\theta) \cdot \cos(m\varphi)$$

or

$$y_{l,m}(\theta) \cdot \sin(m\varphi)$$

where $x = \cos\theta$ & $y_{l,m}(\theta)$ can obey

$$(1-x^2)y'' - 2xy' + \left[l(l+1) - \frac{m^2}{1-x^2}\right]y = 0$$

for $m^2 \leq l^2$

This is called Legendre's associated diff. eq. & reduces to Legendre's diff. eq. if $m = 0$, so that

$$y_{l,m=0}(\theta) = P_l(x)$$

could solve this by using series, but we will just verify the known solution.

First make the substitution

$$y = (1-x^2)^{m/2} u \equiv v^{m/2} u$$

Then $$(v^{m/2})' = \frac{d}{dx}(1-x^2)^{m/2}$$

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

$$= -xm(1-x^2)^{\frac{m}{2}-1}$$

$$= -mx\, v^{m/2-1}$$

& $$(v^{m/2})'' = -m v^{m/2-1} - mx\left[v^{m/2-1}\right]'$$

$$= -m v^{m/2-1} - mx\left(\frac{m}{2}-1\right) v^{m/2-2} \cdot (-2x)$$

$$= -m v^{m/2-1} + m(m-2)x^2 v^{m/2-2}$$

then $$y' = \left[u v^{m/2}\right]' = u' v^{m/2} + u\left[v^{m/2}\right]'$$

$$= u' v^{m/2} + u\left[-mx\, v^{m/2-1}\right]$$

⑩

&

$$y'' = \left[u v^{m/2}\right]''$$

$$= u'' v^{m/2} + 2u'\left[v^{m/2}\right]' + u\left[v^{m/2}\right]''$$

$$= u'' v^{m/2} + 2u'\left[-mx\, v^{m/2-1}\right]$$

$$+ u\left[-m v^{m/2-1} + m(m-2)\, x\, v^{m/2-2}\right]$$

Now plug in to associated Legendre diff. eq.

$$v\left\{u'' v^{m/2} + 2u'(-mx\, v^{m/2-1}) + u\left[-m v^{m/2-1} + m(m-2)\, x\, v^{m/2-2}\right]\right\}$$

$$-2x\left[\quad u' v^{m/2} + u\left[-mx\, v^{\frac{m}{2}-1}\right]\right]$$

$$+\left(\lambda - m^2/v\right) v^{m/2} u = 0$$

$$\Rightarrow u'' v^{(m/2+1)} - 2mxu'v^{m/2} + \left(-mv^{m/2} + m(m-2)x^2 v^{\frac{m}{2}-1}\right)u$$

$$+ \quad -2xu'v^{m/2} + \left(2mx^2 v^{\frac{m}{2}-1}\right)u$$

$$+ \left(\lambda v^{m/2} - m^2 v^{\frac{m}{2}-1}\right)u = 0$$

$$\Rightarrow u'' v^{m/2+1} - 2(m+1)xu'v^{m/2}$$

$$+ \left[(\lambda - m)v^{m/2} + \left(m(m-2)x^2 + 2mx^2 - m^2\right)v^{\frac{m}{2}-1}\right]u = 0$$

$$\Rightarrow v v^{m/2} u'' - 2(m+1)x v^{m/2} u'$$

$$+ \left[(\lambda - m)v^{m/2} + (m^2x^2 - m^2)\ v^{\frac{m}{2}-1}\right]u = 0$$

$$\Rightarrow v v^{m/2} u'' - 2(m+1)x v^{m/2} u'$$

$$+ \left[(\lambda - m)v^{m/2} - m^2 v^{m/2}\right]u = 0$$

Divide by $v^{m/2}$:

$$\Rightarrow (*) \quad vu'' - 2(m+1)xu' + \left[\lambda - m(m+1)\right]u = 0$$

If $m=0$, this reduces to

$$(1-x^2)\, u_0'' - 2x\, u_0' + \lambda u_0 = 0$$

$$\Rightarrow u_{\ell, m=0} = P_\ell(x)$$

Now differentiate previous equation (*) to get

$$v' u'' + v u''' - 2(m+1)\left[u' + x u''\right] + \Big[\lambda - \underbrace{m(m+1)}_{\mu}\Big] u' = 0$$

$$\Rightarrow -2x u'' + \ldots$$

$$\Rightarrow v u''' + \left[-2(m+1)x - 2x\right] u'' + \left[\lambda - \mu - 2(m+1)\right] u' = 0$$

$$\Rightarrow (1-x^2)(u')'' - 2\left[(m+1)+1\right] x\, (u')' + \left[\lambda - \big(m(m+1) + 2(m+1)\big)\right] u' = 0$$

$$\Rightarrow (1-x^2)[u']'' - 2\left[(m+1)+1\right] x [u']' + \left[\lambda - (m+1)(m+2)\right] u' = 0$$

which means that u' is a solution to (#) w/ $m \to m+1$.

i.e.,

$u = P_\ell(x)$ is a solution when $m=0$

$u' = P_\ell'(x)$ . . . . . . $m=1$

$u'' = P_\ell''(x)$ . . . . . . $m=2$

$\vdots$

$u^{(m)} = P_\ell^{(m)}(x)$ . . . . . . $m=m$

$$\Rightarrow u_m = \frac{d^m}{dx^m} P_\ell(x) \qquad \forall \ell, m$$

w/ $$y = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x)$$

Rodrigues formula for associated Legendre

Recalling that

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

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