D1

Differential operators + Sturm-Liouville Theory

Matrices act on vectors $\left\{ \begin{array}{l} \text{eigenvectors} \\ \text{eigenvalues} \\ \text{etc etc} \end{array} \right.$

What acts on functions?

Differential operators

$$\mathcal{L} = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x)$$

$$\mathcal{L}f(x) = p_0(x)f''(x) + p_1(x)f'(x) + p_2(x)f(x)$$

We can ask: What are eigenfunctions (eigenvectors) and eigenvalues of $\mathcal{L}$. Ie what functions obey

$$\mathcal{L}f = \lambda f.$$

Under what conditions are those functions "complete"?
[what is analog of "Hermitian" for $\mathcal{L}$?]

Suppose $\mathcal{L} = d^2/dx^2$ write $\lambda = -n^2$ for convenience

$$d^2/dx^2 \, f = \lambda f = -n^2 f$$

$$f = \sin nx \quad \cos nx$$

If we demand f be periodic with period 2π, n must be integer

So here's a secret of mathematical physics:

Most of the special functions one encounters are eigenfunctions of $\mathcal{L}$ with some choice of p_0, p_1, p_2.

The "famous" ones we know have $p_0\ p_1\ p_2$ which happen to arise from important problems in physics:

Hydrogen atom, EM, ...

Eigenfunctions and Eigenvalues of $\mathcal{L}$?

Natural to ask: Is $\mathcal{L}$ "Hermitian"?

$H_{ij} = H^*_{ji}$ for matrix $H = H^\dagger$

What are "matrix elements" of $\mathcal{L}$?

$$\mathcal{L}_{fg} = \langle f | \mathcal{L} g \rangle = \int_a^b f^*(x) \, \mathcal{L} \, g(x) \, dx$$

$$\text{"Hermitian" if} \quad = \mathcal{L}^*_{gf} = \left(\int_a^b g^*(x) \, \mathcal{L} f(x) \, dx \right)^*$$

We will need to come back to when this is true generally, but for the specific example needed for Fourier analysis...

f, g real

$$\int_0^{2\pi} f\left(\frac{d^2}{dx^2}\right) g = f g' \Big|_0^{2\pi} - \int_0^{2\pi} f' g' \, dx$$

$$= (f g' - f' g)\Big|_0^{2\pi} + \int_0^{2\pi} f'' g \, dx$$

$$\mathcal{L}_{fg} = \underbrace{(f g' - f' g)\Big|_0^{2\pi}}_{\substack{\text{vanishes} \\ \text{for } f,g \text{ periodic on } 2\pi}} + \mathcal{L}_{gf} \qquad \checkmark\checkmark$$

Self Adjointness / Hermiticity

$$\mathcal{L} = p_0 \frac{d^2}{dx^2} + p_1\, d/dx + p_2$$

$\mathcal{L}_{fg} = \langle f | \mathcal{L} g \rangle =$ Let's assume f, g real

$$= \int_a^b dx\; f(p_0 g'' + p_1 g' + p_2 g)$$

$$\mathcal{L}_{gf} = \int_a^b dx\; g(p_0 f'' + p_1 f' + p_2 f)$$

$$= \int_a^b dx\left[-(g p_0)' f' - (g p_1)' f + p_2 f g\right] + (g p_0) f' + g p_1 f \Big|_a^b$$

$$= \int_a^b dx\left[(g p_0)'' f - (g p_1)' f + p_2 f g\right] + (g p_0) f' + g p_1 f \Big|_a^b$$

$$- (g p_0)' f \Big|_a^b$$

$$(g p_0)'' = (g' p_0 + g p_0')' = g'' p_0 + 2 g' p_0' + g p_0''$$

$$\mathcal{L}_{gf} = \int_a^b dx\left[\left(\cancelto{a}{g'' p_0} + 2 g' p_0' + g p_0''\right) f - (g' p_1 + g p_1') f + \cancelto{b}{p_2 f g}\right]$$

$$+ \left[g p_0 f' + g p_1 f - (g p_0)' f\right]_a^b$$

$$\mathcal{L}_{fg} = \int_a^b dx\left[f\, \cancelto{a}{p_0 g''} + f p_1 g' + f \cancelto{b}{p_2 g}\right]$$

Integrands: $\quad f(2p_0' - p_1) g' + f(p_0'' - p_1') g = f p_1 g'$

$$2 f (p_0' - p_1) g' + f (p_0'' - p_1') g = 0$$

So Hermiticity is guaranteed if

$$p_1 = p_0'$$

and

what about bdy term?

$$\left. g p_0 f' + \cancel{g p_1 f} - \underbrace{(g p_0)' f}_{-g' p_0 f - \cancel{g p_0' f}} \right|_a^b$$

ami: $(a,b) = (-\infty, \infty)$

$$\left. p_0 (g f' - g' f) \right|_a^b = 0$$

(1) Dirichlet bdy conditions : f, g vanish at endpoints a, b

(2) Neumann bdy conditions : f', g' " " " " "

(3) Periodic bdy condition : $f(a) = f(b)$; $f'(a) = f'(b)$ + similarly for g.

$$\mathcal{L} = p_0 \frac{d^2}{dx^2} + p_0' \frac{d}{dx} + p_2$$

$$= \frac{d}{dx}\left(p_0 \frac{d}{dx}\right) + p_2$$

(56)

"weight function"

$$\mathcal{L} u(x) = \lambda w(x) u(x)$$

Generalized eigenvalue problem
$M\vec{v} = \lambda R \vec{v}$
(eg LAPACK)

Why? Consider s.h.o.

$$\underbrace{\left[-\hbar^2/2m \frac{d^2}{dx^2} + 1/2\, m\omega^2 x^2\right]}_{\mathcal{L}} \psi(x) = \lambda \psi(x)$$

Is $\mathcal{L}$ Hermitian? Yes! $p_0 = -\frac{\hbar^2}{2m}$ $\quad p_0' = 0 = p_1$

Try power series soln

Define $\quad \psi(x) = e^{-m\omega/2\hbar\, x^2}\, v(x)$

Recursion reln for $v(x)$ is more simple than for $\psi(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[e^{-m\omega x^2/2\hbar}\, v\right]$$

$$= -\frac{\hbar^2}{2m}\frac{d}{dx}\left[-\frac{m\omega}{\hbar} x e^{-m\omega x^2/2\hbar} v + e^{-m\omega x^2/2\hbar} v'\right]$$

$$= -\frac{\hbar^2}{2m}\left[\frac{m^2\omega^2}{\hbar^2} x^2 v - \frac{m\omega}{\hbar} e^{-m\omega x^2/2\hbar} v - 2\frac{m\omega}{\hbar} x e^{-m\omega x^2/2\hbar} v'\right.$$

cancels potential term

$$\left. - e^{-m\omega x^2/2\hbar} v''\right]$$

So $\quad \mathcal{L}\left[e^{-m\omega x^2/2\hbar} v\right]$

note no p_2 term!

$$= \left[\frac{\hbar^2}{2m} e^{-m\omega x^2/2\hbar}\frac{d^2}{dx^2} + \hbar\omega x e^{-m\omega x^2/2\hbar}\frac{d}{dx}\right] v(x)$$

$$= \left[\lambda - \frac{\hbar\omega}{2}\right] e^{-m\omega x^2/2\hbar}\, v(x)$$

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Check Hermiticity in this form:

$$P_1(x) = 1/\omega \; d/dx \; \omega \; P_0(x)$$

$\hbar\omega x e^{-m\omega^2 x^2/2\hbar}$

$\frac{\hbar^2}{2m} \underbrace{e^{-m\omega^2 x^2/2\hbar} \quad e^{-m\omega^2 x^2/2\hbar}}$

$e^{-m\omega^2 x^2/\hbar}$

$\frac{m\omega^2 x}{\hbar}$

$\hbar\omega x$

$v(x) = 1 \qquad \lambda = +\hbar\omega/2$

57

Hermiticity condition slightly different when w is present!

$$p_1(x) = 1/w \; d/dx \, (w p_0)$$

Here $$= e^{+m\omega x^2/2\hbar} \, d/dx \left[e^{-m\omega x^2/2\hbar} \frac{\hbar^2}{2m} e^{-m\omega x^2/2\hbar} \right]$$

$$= e^{+m\omega x^2/2\hbar} \frac{\hbar^2}{2m} \frac{2m\omega x}{\hbar} e^{-m\omega x^2/\hbar}$$

$$= \hbar \omega x e^{-m\omega x^2/2\hbar} \quad \checkmark\checkmark$$

Recall $p_1(x) = p_0'(x)$

	$p_0(x)$	$p_2(x)$	$w(x)$
Fourier	1	$\emptyset$	1
Legendre	$(1-x^2)$	$\emptyset$	1
Hermite	e^{-x^2}	$\emptyset$	e^{-x^2}
Bessel	x	$-n^2/x$	x
Laguerre	xe^{-x}	$\emptyset$	e^{-x}
Chebyshev	...		
Gegenbauer			
⋮			

$\boxed{\text{ch 9 \quad Table 9.1}}$

Matrix ≡ PDE

Sch = Heisenberg

* Again emphasize all these special functions can be regarded as eigenfunctions of particular Hermitian 2nd order differential operators

weight $\int_a^b f(x)\, g(x)\, w(x) = 0$

f, g different λ

Hermiticity is true $\int_a^b f \mathcal{L} g = \int_a^b g \mathcal{L} f$