Sturm - Liouville Theory

1. L^p Space

We can notice that all the integrable functions could form a linear space. Now, could we set up norm for the space?

At the first glance, we have

$$\|f\|_{L^p} = \left(\int_X |f(x)|^p dx\right)^{\frac{1}{p}} \quad (\text{we only consider } f \text{ such that } \|f\|_{L^p} < \infty)$$

But there's some problems: imagine that there's two functions: $\varphi(x)$ and $\psi(x)$. They have different values at the points which belong to zero measure set (the points are countable if infinite). Now they could have the same norm, unless $p=\infty$. As a result, $\|f\|_{L^p}=0$ doesn't mean that $f=0$. However, we can introduce the equivalence ~~of~~ classes, in which f and g are the same thing if $\|f\|_{L^p} = \|g\|_{L^p}$.

*. What if $p \to \infty$?

* How to prove that $\|f\|_{L^p}$ is norm (if we take equivalence classes into account?)

hint: Minkowski Inequalities

Theorem: The space L^p is complete in the norm $\|\cdot\|_{L^p}$

Now the space is complete, which is important for us to find the series (Usually, we choose $p=2$)

2. Inner product

2.1 Definition:

$\langle x_1, x_2 \rangle = \overline{\langle x_2, x_1 \rangle}$

$\langle x_0, \lambda x_1 + \beta x_2 \rangle = \lambda \langle x_0, x_1 \rangle + \beta \langle x_0, x_2 \rangle$

$\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0$ iff $x = 0$

From the definition, we can define norm for the space. We can guass that $\|x\| = \sqrt{\langle x, x \rangle}$ (from R^n)

as $\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0$ iff $x=0$, we have

$\|x\| \geq 0$ and $\|x\| = 0$ iff $x = 0$

and $\|\lambda x\| = \sqrt{\langle \lambda x, \lambda x \rangle} = \sqrt{\lambda \lambda^* \langle x, x \rangle} = |\lambda| \|x\|$.

As for $\|x_1 + x_2\| \leq \|x_1\| + \|x_2\|$, we should introduct: $|\langle x, y \rangle|^2 \leq \langle x, x \rangle \langle y, y \rangle$

We have ~~$\langle x + \lambda y \rangle \langle \rangle$~~

$\langle x + \lambda y, x + \lambda y \rangle \geq 0$, and $a = \langle x, x \rangle$ $c = \langle y, y \rangle$, $b = \langle x, y \rangle$

Thus, $|b|^2 \leq ac$, and $|\langle x, y \rangle|^2 \leq \langle x, x \rangle \langle y, y \rangle$

From that, we can get

$(\langle x+y, x+y \rangle)^{\frac{1}{2}} \leq (\langle x, x \rangle)^{\frac{1}{2}} + (\langle y, y \rangle)^{\frac{1}{2}}$, just as norm

So Hilbert space is always Banach space.

Notice that we have proved the completeness of norm in L^P. Now we can introduce the inner product in L^P. Usually we take $p=2$, and as a result, $\langle f, g\rangle = \int_X f^*(x) g(x) dx$.

Since the norm generated by $\langle f, g\rangle$ is $\|f\|_{L^2}$, which is complete, we can conclude that the space is Hilbert space.

So now it is possible to set up a complete series to generate all the elements in L^P.

※. The completeness of the series is restricted to the equivalence classes.

2.2 Weighted Orthogonal

Notice that we can generate a new L^2 space V' using the L^2 space V and the function whose value is always positive $(p(x))$.

We set that $V' := \{\sqrt{p(x)}\, f(x) \mid f(x) \in V\}$, so naturally we have inner product $\langle f, g\rangle = \int_X p(x) f^*(x) g(x) dx$.

And we define f and g to be orthogonal if $\langle f, g\rangle = 0$

3. Expansions in Orthogonal Systems of Functions

(Generalized Fourier Series)

If the series is complete, they it would be possible for us to expand the function to the series without losing any information.

Now we'd like to learn the expansions in orthogonal systems. When it comes to finite dimensions, it's obvious that

$$x = \frac{\overline{\langle x, l_1\rangle}}{\langle l_1, l_1\rangle} l_1 + \frac{\overline{\langle x, l_2\rangle}}{\langle l_2, l_2\rangle} l_2 + \dots + \frac{\overline{\langle x, l_n\rangle}}{\langle l_n, l_n\rangle} l_n = \frac{\langle l_1, x\rangle}{\langle l_1, l_1\rangle} l_1 + \dots + \frac{\langle l_n, x\rangle}{\langle l_n, l_n\rangle} l_n$$

When it comes to infinite dimensions, it should be the same. If

$$x = \sum_{i=1}^{\infty} a_i \frac{\overline{\langle x, l_i\rangle}}{\langle l_i, l_i\rangle} l_i = \sum_{i=1}^{\infty} \frac{a_i \langle l_i, x\rangle l_i}{\langle l_i, l_i\rangle} \text{ (} l_i \text{ is complete)}$$

Then

$$\langle l_{i_0}, x\rangle = \sum_{i=1}^{\infty} \frac{a_i \langle l_i, x\rangle}{\langle l_i, l_i\rangle} \langle l_{i_0}, l_i\rangle = \sum_{i=1}^{\infty} a_i \langle l_i, x_0\rangle \delta_{i i_0} = a_i \langle l_{i_0}, x\rangle$$

$$\therefore a_i = 1, \text{ and } x = \sum_{i=1}^{\infty} \frac{\langle l_i, x\rangle}{\langle l_i, l_i\rangle} l_i$$

Now we take use of the definition of inner product in L^2:

$\langle f, g\rangle = \int_X \rho(x) f^*(x) g(x) dx$, we have

$$f(x) = \sum_{i=1}^{\infty} \frac{\int_X \rho(x) l_i^*(x) f(x) dx}{\int_X \rho(x) l_i^*(x) l_i(x) dx} l_i(x)$$

Now we call $\sum_{i=1}^{\infty} \frac{\langle l_i, x\rangle}{\langle l_i, l_i\rangle} l_i$ Fourier Series (in the orthogonal system $\{l_k\}$)

Then we will study the completeness: where the equity could hold.

Lemma: If Fourier Series of x in the system $\{l_k\}$ converges to x_L, then $h = x - x_L$ is orthogonal to x_L, and h is orthogonal to the entire linear subspace of $\{l_k\}$ and its closure (added all the limit points)..

(The proof is obvious)

Notice that if $\langle a, b\rangle = 0$, then $\|a+b\|^2 = \|a\|^2 + \|b\|^2$

Thus, $\|x\|^2 = \|x_L\|^2 + \|h\|^2$, and $\|x_L\|^2 = \sum_k \left|\frac{\langle l_k, x\rangle}{\langle l_k, l_k\rangle}\right|^2 \langle l_k, l_k\rangle = \sum_k \frac{|\langle l_k, x\rangle|^2}{\langle l_k, l_k\rangle}$

So we can get Bessel's Inequality: $\|x\|^2 \geq \sum_k \frac{|\langle l_k, x\rangle|^2}{\langle l_k, l_k\rangle} = \sum_k |\langle e_k, x\rangle|^2$

4. Completeness

We say the system $\{x_\alpha;\ \alpha \in A\}$ is complete in $E \subset X$ if every vector $x \in E$ can be approximated with arbitary accuracy in the sense of norm of X by finite linear combinations of x_α.

Or to say, $E \subseteq \overline{L}\{x_\alpha\}$ (closure)

And those below are equivalent

(a) $\{l_k\}$ is complete with respect to set $E \subset X$

(b) for every vector $x \in E$, $x = \sum_k \frac{\langle l_k, x\rangle}{\langle l_k, l_k\rangle} l_k$

(c) for every vector $x \in E \subset X$,

$$\|x\|^2 = \sum_k \frac{|\langle l_k, x\rangle|^2}{\langle l_k, l_k\rangle} \quad \text{(Parseval's equality)}$$

If $E=X$, and the space X is complete, then X contains no non zero vector orthogonal to all vectors in the system $\{l_k\}$ will be sufficient condition for $\{l_k\}$ to complete.

And it's always ~~nessary~~ necessary condition.

5. Sturm - Liouville Theory

We call the equation

$$\frac{d}{dx}\left[k(x)\frac{dy}{dx}\right] - q(x)y + \lambda p(x)y = 0 \quad (a \le x \le b)$$

Sturm - Liouville Equation.

And it could have boundary conditions.

*. natural conditions: no divergence

for usuall equations

$y''(x) + ay' + by + \lambda cy = 0$, we multiply them with $\exp(\int a(x)dx)$,

and there's $\frac{d}{dx}\left[e^{\int a(x)dx}\frac{dy}{dx}\right] + b(x)e^{\int a(x)dx}y + \lambda\left[c(x)e^{\int a(x)dx}\right]y = 0$

So it's general problem

Usually we set $k(x)$, $q(x)$ and $p(x) \geq 0$, and then we have
(They are real)

The Properties:

(1) If $k(x)$, $k'(x)$ and $q(x)$ are continuous or has first order pole at $x=a$ or $x=b$, there would be infinite eigenvalue

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq \cdots$$

and eigenfunctions as well

$$y_1(x), y_2(x) \cdots y_n(x) \cdots$$

(2) all the eigenvalue $\lambda_n \geq 0$.

Proof: as $-\frac{d}{dx}[k(x)\cdot\frac{dy_n}{dx}] + q(x)y_n = \lambda_n \rho(x)\cdot y_n$

we have $\lambda_n \rho(x) y_n^2 = -y_n\frac{d}{dx}[k(x)\frac{dy_n}{dx}] + q(x) y_n^2$

Thus, $\lambda_n \int_a^b \rho(x) y_n^2 dx = \int_a^b q y_n^2 dx - \int_a^b y_n \frac{d}{dx}[k(x)\frac{dy_n}{dx}]\cdot dx$

$$= -[k y_n \frac{dy_n}{dx}]\Big|_a^b + \int_a^b k(\frac{dy_n}{dx})^2 dx + \int_a^b q y_n^2 dx$$

$$= (k y_n y_n')_{x=a} - (k y_n y_n')_{x=b} + \int_a^b q y_n^2 dx + \int_a^b k y_n'^2 dx$$

Notice that $\int_a^b q y_n^2 dx + \int_a^b k y_n'^2 dx \geq 0$, $\int_a^b \rho(x) y_n^2 dx = 0$

If $y_n(a)=0$ (Dirichlet Boundary Condition) or $y_n'(a)=0$ (Neumann Boundary condition) or $k(a)=0$ (natural),

then $(k y_n y_n')_{x=a} = (k y_n y_n')|_{x=b} = 0$

If it's the third boundary condition $(y_n - h y_n')_{x=a} = 0$,

Then $(k y_n y_n')_{x=a} = (hk y_n'^2)_{x=a} \geqslant 0$

for b: if $(y_n + h y_n')_{x=b} = 0$, Then $-(k y_n y_n')_{x=b} \geqslant 0$

As a result, $\lambda_n \geqslant 0$

(3) if $\lambda_m \neq \lambda_n$, then $y_m(x)$ and $y_n(x)$ related to λ_m and λ_n are orthogonal on $[a,b]$ with weight $\rho(x)$: $\int_a^b y_m(x) y_n(x) \rho(x) dx = 0$ $(m \neq n)$ (real)

or $\int_a^b y_m^*(x) y_n(x) \rho(x) dx = 0$ (complex)

Proof: we have $\frac{d}{dx}[k y_m'] - q y_m + \lambda_m \rho y_m = 0$

from (1), we can know tham $\lambda_m \geqslant 0$ $\therefore \lambda_m \in R$

$\therefore \frac{d}{dx}[k y_m^{*\prime}] - q y_m^* + \lambda_m \rho y_m^* = 0$

and $\frac{d}{dx}[k y_n'] - q y_n + \lambda_n \rho y_n = 0$

Thus, $(\lambda_m - \lambda_n) \rho y_m^* y_n = y_m^* \frac{d}{dx}[k y_n'] - y_n \frac{d}{dx}[k y_m^{*\prime}]$

$= \frac{d}{dx}(k y_m^* y_n' - k y_m^{*\prime} y_n)$

$\therefore (\lambda_m - \lambda_n) \int_a^b \rho y_m^* y_n dx = (k y_m^* y_n' - k y_n^* y_m') \Big|_{x=a}^{x=b}$

We now get boundary condition into the right part of equation, and it's 0.

Notice that $\lambda_m - \lambda_n \neq 0$ $\therefore \int_a^b \rho y_m^* y_n dx = 0$

(4) The series $y_1(x), y_2(x) \cdots$ is complete.

If $f(x)$ is continuous and $f''(x)$ is piecewise continuous,

then $f(x) = \sum_{n=1}^{\infty} f_n y_n(x)$, which is absolute and uniform convergence.

($f(x)$ is continuous, so the equivalence classes ~~have~~ have only 1 function in each of them)

Here $f_n = \frac{1}{N_n^2} \int_a^b y_n^*(x) \rho(x) f(x) dx$,

$N_n^2 = \int_a^b \rho(x) y_n^*(x) y_n(x) dx$

Example: Laguerre Polynomials:

$xy'' + (1-x) y' + \lambda y = 0 \quad (0 < x < \infty)$ is called Laguerre Equation

That could be transformed into:

$\frac{d}{dx}[x e^{-x} \frac{dy}{dx}] + \lambda e^{-x} y = 0$

That's to say, $\int_0^{\infty} L_m(x) L_n(x) e^{-x} dx = 0 \quad (m \neq n)$

Here, the solution $L_n(x) = e^{x} \frac{d^n}{dx^n} (x^n e^{-x})$

*. prove that $L_n(x)$ is the solution to Laguerre Equation

Hint: $\begin{cases} z = x^n e^{-x} \\ x z' + (x-n) z = 0 \end{cases}$

When it comes to series solution, there's

$$y(x) = a_0\left[1 + \frac{-\lambda}{(1!)^2}x + \frac{(-\lambda)(1-\lambda)}{(2!)^2}x^2 + \cdots + \frac{(-\lambda)(1-\lambda)\cdots(k-1-\lambda)}{(k!)^2}x^k + \cdots\right]$$

(convergence radius: ∞)

If λ is integar, then $y(x)$ is polynomials (Laguerre polynomials)

(Notice that $y(x) \sim e^x$ if λ isn't integar, which is contradictory with $\int |\Psi|^2 dr^3 = 1$)

And we have

$$\int_0^{+\infty} [L_n(x)]^2 e^{-x} dx = \int_0^{+\infty} \frac{d^n}{dx^n}(x^n e^{-x}) \cdot \left[e^x \frac{d^n}{dx^n}(x^n e^{-x})\right] dx$$

$$= -\int_0^{+\infty} \frac{d^{n-1}}{dx^{n-1}}(x^n e^{-x}) \cdot \left[\frac{d}{dx}\left(e^x \frac{d^n}{dx^n}(e^{-x} x^n)\right)\right] dx$$

$$= \cdots$$

$$= (-1)^n \cdot \int_0^{+\infty} x^n e^{-x} \frac{d^n}{dx^n}\left(e^x \frac{d^n}{dx^n}(x^n e^{-x})\right) dx$$

Notice that $\frac{d^n}{dx^n}\left(e^x \frac{d^n}{dx^n}(x^n e^{-x})\right) = \frac{d^n}{dx^n} \cdot [(-1)^n \cdot x^n e^x \cdot e^{-x}] = (-1)^n \cdot n!$

Thus, $\int_0^{+\infty} e^{-x} [L_n(x)]^2 dx = \int_0^{+\infty} n! x^n e^{-x} dx = (n!)^2$

Example: Hermite Polynomial

Hermite Equation: $y'' - 2xy' + \lambda y = 0 \quad (-\infty < x < +\infty)$

That is to say, $\frac{d}{dx}[e^{-x^2}\frac{dy}{dx}] + \lambda e^{-x^2} y = 0$

and $\int_{-\infty}^{+\infty} H_m(x) H_n(x) e^{-x^2} dx = 0 \ (m \neq n)$

For series solution, there would be

$$y_0(x) = 1 + \frac{-\lambda}{2!}x^2 + \frac{(-\lambda)\cdot(4-\lambda)}{4!}x^4 + \cdots + \frac{(-\lambda)(4-\lambda)\cdots(4n-4-\lambda)}{4!}x^{2n} + \cdots$$

$$y_1(x) = x + \frac{2-\lambda}{3!}x^3 + \cdots + \frac{(2-\lambda)(6-\lambda)\cdots(4n-2-\lambda)}{(2n+1)!}x^{2n+1} + \cdots$$

(convergence radius: ∞)

If $\lambda = 4n$ ($n \in N^*$), then $y_0(x)$ would become $\frac{1}{2}\lambda$-order polynomial; If $\lambda = 4n-2$ ($n \in N^*$), y_1 would become $\frac{1}{2}\lambda$-order polynomial. That's Hermite Polynomial. That's $N_m = (-1)^m \cdot e^{x^2}\frac{d^m}{dx^m}(e^{-x^2})$

(Only at that time could $\int |\Psi|^2 dv$ be satisfied).

As for N_m^2, there is

$$\int_{-\infty}^{+\infty} [H_m(x)]^2 e^{-x^2} dx = \int_{-\infty}^{+\infty} \frac{d^m}{dx^m}(e^{-x^2}) \cdot [e^{x^2}\frac{d^m}{dx^m}(e^{-x^2})] dx$$

$$= \cdots = \int_{-\infty}^{+\infty} (-1)^m e^{-x^2} \frac{d^m}{dx^m}[e^{x^2}\frac{d^m}{dx^m}(e^{-x^2})] dx$$

Notice that $\frac{d^m}{dx^m}[e^{x^2}\frac{d^m}{dx^m}(e^{-x^2})] = (-2)^m \frac{d^m}{dx^m} \cdot x^m = (-2)^m \cdot m!$

$\therefore \int_{-\infty}^{+\infty} [H_m(x)]^2 e^{-x^2} dx = 2^m \cdot m! \int_{-\infty}^{+\infty} e^{-x^2} dx = 2^m m! \sqrt{\pi}$

6. The Relation Between Sturm–Liouville Theory and Hermite Operators

(1) S-L depends on the range of x and boundary condition, while Hermite doesn't.

(2) Hermite is more abstract ($F^{+}=F$, ~~ank~~ and $-i\hbar\frac{\partial}{\partial x}$, x ... are all ok). and $\frac{d}{dx}[k(x)\frac{d}{dx}]-q(x)$ is more specific

(3) S-L theory has weight function, while for Hermite, $\rho(x)=1$

(4) While expanding $f(x)$, S-L theory requires $f(x)$ to have the same boundary condition, while Hermite operator doesn't

(It's not absolute)

Varation Method

We know that if $|\psi\rangle$ isn't normalized, there will be

$$H = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$ and we know that $H \geq E_0$ (ground state)

So ~~A~~ a mong all the function families, $E = E(\alpha, \beta \cdots)$,

E_0 would be one of $E_{min} = E(\alpha_0, \beta_0 \cdots)$. But there are too many families. What should we do?

In fact, we should choose the function family that could maintain the properties of ground state (parity, minimize V, etc.)

Example: $V = \lambda x^4$, we chose

$$\psi(x, \alpha) = \exp\left(-\frac{\alpha x^2}{2}\right)$$ (no need for normalize)

$$\therefore E(\alpha) = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int e^{-\frac{\alpha x^2}{2}} \cdot \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \lambda x^4\right) e^{-\frac{\alpha x^2}{2}} dx}{\int e^{-\alpha x^2} dx}$$

$$= \frac{\hbar^2 \alpha}{4m} + \frac{\cancel{4\lambda}\, 3\lambda}{4\alpha^2}$$

$$\therefore \text{when } \alpha_0 = \left(\frac{6m\lambda}{\hbar^2}\right)^{\frac{1}{3}}, \quad E(\alpha_0) = \frac{3}{8}\left(\frac{6\hbar^4\lambda}{m^2}\right)^{\frac{1}{3}}$$

And at least, $0 \leq E_0 \leq E(\alpha_0)$

advantage: More accurate for ground state

assume that $|\psi\rangle = |E_0\rangle + \delta|E_1\rangle$

Then $E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{E_0 + \delta^2 E_1}{1+\delta^2} = E_0 + k\delta^2 E_1$

$= E_0 + O(\delta^2)$

Normalization: 1 or δ?

If it's discrete, then from $|\psi\rangle = \sum \frac{\langle\varphi_n|\psi\rangle}{\langle\varphi_n|\varphi_n\rangle}|\varphi_n\rangle$, it should be 1

$\langle\varphi_n|\varphi_n\rangle = 1$, and $|\psi\rangle = \sum \langle\varphi_n|\psi\rangle|\varphi_n\rangle$

But what if it is continuous? Notice that it's not ~~countd~~ countable. If $\langle\varphi_n|\varphi_n\rangle$ isn't ∞, then given

$\langle\psi|\psi\rangle = \sum \frac{|\langle\varphi_n|\psi\rangle|^2}{\langle\varphi_n|\varphi_n\rangle}$, and from a restricted interval, there's more number than natural number, so it's infinite, which isn't possible.

Notice that $\int \delta \cdot dx = 1$, so whether we can normalize it to 1?

Yes! And Given $\int \delta(x-x_0)\,dx = 1$,

we have $|\psi\rangle = \int |\varphi\rangle\langle\varphi|\psi\rangle dx = \int |\varphi(x)\rangle\langle\varphi(x)|\psi\rangle dx$