Chapter 6

Some basis of functions

6.1 Sturm-Liouville eigenvalue problems

6.1.1 Scalar product

Let w be a weight function, $w(x) \geq 0$, defined over the support $S = [a, b]$ with possibly $a = -\infty$ and/or $b = \infty$. Let u and v two real functions, one defines the scalar product with respect to w, denoted by $\langle .|. \rangle_w$, as

$$\langle v|u \rangle_w = \int_a^b v(x)u(x)w(x)dx \tag{6.1}$$

where $d\mu(x) = w(x)dx$ is called the measure of integration. The notation $\langle v|u \rangle$ stands for $w = 1$ or corresponds to cases where there is no ambiguity in the presence of w.

Consider that you have a complete set (basis) of orthogonal functions $\{f_n(x)\}$ with respect to $\langle .|. \rangle_w$. Then one can expand any function over S as

$$f(x) = \sum_n \frac{\langle f_n|f \rangle_w}{\langle f_n|f_n \rangle_w} f_n(x) \tag{6.2}$$

6.1.2 Linear operator for Sturm-Liouville

Consider the following differential eigenvalue problem $\hat{L}y = -\lambda y$ (sign is a convention) defined on S with $y(x)$ a real function that satisfies to given boundary conditions. We assume that $\hat{L}$ is a linear second-order differential operator of the form

$$\hat{L} = p(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)\frac{\mathrm{d}}{\mathrm{d}x} + m(x) \tag{6.3}$$

where p, q, m are continuous functions and p' exists and is also continuous.

A sufficient condition for $\hat{L}$ to be hermitian (self-adjoint) with respect to the unweighted scalar product $\langle .|. \rangle$ (i.e. $\langle v|\hat{L}u \rangle = \langle \hat{L}v|u \rangle$) is that $p' = q$ and that the boundary terms $[p(vu' - v'u)]_a^b = 0$ vanish, in which case one has:

$$\hat{L} = \frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + m(x)\ . \tag{6.4}$$

6.1.3 Making the operator Hermitian

Starting from a non-hermitian operator $\hat{L}$, one can introduce a weight function w such that $\hat{H} = w\hat{L}$ is hermitian with respect to the *weighted* scalar product $\langle .|. \rangle_w$ and provided the boundary terms $[wp(vu' - v'u)]_a^b = 0$ vanish. The form of w is given by:

$$w(x) = \frac{1}{p(x)} \exp\left\{\int^x \frac{q(x')}{p(x')}dx'\right\}. \tag{6.5}$$

The required boundary conditions also ensures orthogonality of non-degenerate eigenfunctions.

6.1.4 Spectral theorem for regular Sturm-Liouville problems

A Sturm-Liouville problem put in the form $\hat{H}y = -\lambda wy$ is regular if: S is a finite interval (confinement), $p(x) > 0$ and $w(x) > 0$, we have boundary conditions

$$c_1 y(a) + c_2 y'(a) = 0 \quad \text{and} \quad d_1 y(b) + d_2 y'(b) = 0 \quad (c_1, c_2) \neq (0,0), (d_1, d_2) \neq (0,0), \ . \tag{6.6}$$

In this case:

(i) eigenvalues λ_n are real and can be sorted in ascending manner: $\lambda_0 < \lambda_1 < \lambda_2 < \dots$

(ii) eigenfunctions $y_n(x)$ are non-degenerate and have $n-1$ zeros in S.

(ii) eigenfunctions $\{y_n(x)\}$ form an orthogonal basis with respect to the $\langle .|.\rangle_w$ scalar product.

Rk: if the support S is unbounded, degenerate and continuous eigenvalues can exist.

6.2 Orthogonal polynomials

6.2.1 Definition and notations

We assume that the weight function w is such that $\int_a^b x^m w(x)dx$ converges for all $m \in \mathbb{N}$, and we use it to define a scalar product. A set of polynomials $\{P_n(x)\}$ is orthogonal with respect to w if $\langle P_n|P_{n'}\rangle_w = N_n \delta_{nn'}$, with $N_n = \|P_n\|_w^2 = \langle P_n|P_n\rangle_w$.
In what follows, n stands for the order (degree) of the polynomial. Any polynomial P of degree m can then be decomposed as

$$P(x) = \sum_{n=0}^{m} \frac{\langle P_n|P\rangle_w}{\langle P_n|P_n\rangle_w} P_n(x) \ , \tag{6.7}$$

i.e. on the subbasis of polynomials of degrees $n \leq m$.

6.2.2 Recurrence relation

Let $\{P_n(x)\}$ be a set of orthogonal polynomials, there exists three series of coefficients A_n, B_n, C_n such that for $n \geq 1$:

$$xP_n(x) = A_n P_{n+1}(x) + B_n P_n(x) + C_n P_{n-1}(x) \tag{6.8}$$

with $A_n C_n \neq 0$. Let a_k^n be the coefficients of P_n, ie

$$P_n(x) = \sum_{k=0}^{n} a_k^n x^k \tag{6.9}$$

Then, we have

$$A_n = \frac{a_n^n}{a_{n+1}^{n+1}}, \quad B_n = \frac{a_{n-1}^n}{a_n^n} - \frac{a_n^{n+1}}{a_{n+1}^{n+1}}, \quad C_n = \frac{a_{n-1}^{n-1}}{a_n^n}\frac{N_n}{N_{n-1}} \tag{6.10}$$

6.2.3 Generating function

Let $G(x,t)$ be an analytic function over domain $t \in \mathcal{D}$, it is the generating function of the $\{P_n(x)\}$ family when the $P_n(x)$ are derived by taking the n^{th} derivative of G with respect to t. We don't give a generic definition because it varies from one set to another, basically by an n-dependent prefactor.

6.3 Classical orthogonal polynomials

We consider a special where the orthogonal polynomials are eigenfunctions of a simple (possibly regular) Sturm-Liouville problem.

6.3.1 General structure: Rodrigues formula

We start from the following Sturm-Liouville problem:

$$p(x)y''(x) + q(x)y'(x) + \lambda y(x) = 0 \tag{6.11}$$

in which we choose $p(x)$ and $q(x)$ to be polynomials of second and first order respectively, i.e.

$$p(x) = \alpha x^2 + \beta x + \gamma \text{ and } q(x) = \mu x + \nu \tag{6.12}$$

Clearly, looking for polynomial solutions by inserting a polynomial into the equation will work if one solves for the recurrence relations between the coefficients. In particular, looking at the highest coefficient of a polynomial of degree n provides the eigenvalues:

$$\lambda_n = -\alpha n(n-1) - \mu n \tag{6.13}$$

The eigenfunctions are polynomials $\{P_n\}$ that are orthogonal with respect to the $\langle .|.\rangle_w$ scalar product, in which the weight function is given by (6.5).
The **Rodrigues formula** allows one to extract these polynomials as

$$P_n(x) = c_n \frac{1}{w(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(w(x)p(x)^n\right) \tag{6.14}$$

where c_n is some coefficient that is chosen by convention. This relation allows one to construct the generating function and then to obtain easily the recurrence relation. Otherwise, all properties (orthogonality, recurrence relation, eigenvalues, coefficients,...) can be derived/cross-checked by hand.

6.3.2 Legendre $P_n(x)$

Differential equation	$(1-x^2)y''(x) - 2xy'(x) + n(n+1)y(x) = 0$
Rodrigues formula: $w(x) = 1$	$P_n(x) = \frac{(-1)^n}{2^n n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n}(1-x^2)^n$
Parameters	$S = [-1, 1]\,, \quad \lambda_n = n(n+1)\,, \quad c_n = \frac{(-1)^n}{2^n n!}\,, \quad N_n = \frac{2}{n+1}$
Generating function	$G(x,t) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x)t^n$
Recurrence relation	$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$

6.3.3 Laguerre $L_n(x)$

Differential equation	$xy''(x) + (1-x)y'(x) + ny(x) = 0$
Rodrigues formula: $w(x) = e^{-x}$	$L_n(x) = \frac{e^x}{n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(x^n e^{-x}\right)$
Parameters	$S = [0, \infty[\,, \quad \lambda_n = n\,, \quad c_n = \frac{1}{n!}\,, \quad N_n = 1$
Generating function	$G(x,t) = \frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x)t^n$
Recurrence relation	$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x)$

6.3.4 Hermite $H_n(x)$

Differential equation	$y''(x) - 2xy'(x) + 2ny(x) = 0$
Rodrigues formula: $w(x) = e^{-x^2}$	$H_n(x) = (-1)^n e^{x^2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}e^{-x^2}$
Parameters	$S =]-\infty, \infty[\,, \quad \lambda_n = 2n\,, \quad c_n = (-1)^n\,, \quad N_n = 2^n n!\sqrt{\pi}$
Generating function	$G(x,t) = e^{-t^2+2tx} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$
Recurrence relation	$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$

6.3.5 Chebyschev $T_n(x)$

Differential equation	$(1-x^2)y''(x) - xy'(x) + n^2y(x) = 0$
Rodrigues formula: $w(x) = 1/\sqrt{1-x^2}$	$T_n(x) = \frac{(-1)^n}{(2n-1)!!}(1-x^2)^{1/2}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(1-x^2)^{n-1/2}$
Parameters	$S = [-1, 1]\,, \quad \lambda_n = n^2\,, \quad c_n = \frac{(-1)^n}{(2n-1)!!}\,, \quad N_0 = \pi, N_{n\neq 0} = \frac{\pi}{2}$
Generating function	$G(x,t) = \frac{1-t^2}{1-2xt+t^2} = T_0(x) + 2\sum_{n=1}^{\infty} T_n(x)t^n$
Recurrence relation	$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$

6.4 Bessel functions

Not treated: they are not polynomials but have many common features with classical polynomials: solution of a Sturm-Liouville problem (associated to the Laplacian in cylinder coordinates), orthogonal basis of function associated to the weight function $w(\rho) = \rho$, they have simple generating function and recurrence relations…

✍ ***Exercise 6.1 Darboux-Christoffel formula***
Show that a set of orthogonal polynomials satisfy to the relation:

$$\sum_{k=0}^{n} \frac{1}{N_k} P_k(x) P_k(y) = \frac{1}{N_n} \frac{a_n^n}{a_{n+1}^{n+1}} \frac{P_{n+1}(x) P_n(y) - P_n(x) P_{n+1}(y)}{x - y} \tag{6.15}$$

✍ ***Exercise 6.2 Generating function of Legendre polynomials***

1. Starting from the Rodrigues formula, find the expression of the generating function of Legendre polynomials.
2. Infer the multipole expansion of $1/R$ in powers of a/r and polynomials of $\cos\theta$ in the geometry sketched below

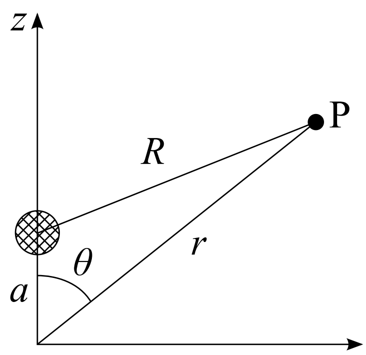

Figure 6.1: Multipole expansion: definition of variables

3. From the generating function, infer the recurrence relation for Legendre polynomials.

✍ ***Exercise 6.3 Recurrence relation of Hermite polynomials***
Using the generating function $G(x, t)$, prove the recurrence relation of the Hermite polynomials.