Orthogonal polynomials

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1.1 Hilbert spaces

Let $\mathcal{V}$ be a vector space equipped with a scalar product $v, w \mapsto (v|w)$. It has then the norm $\|v\| := (v|v)^{\frac{1}{2}}$.We say that $\mathcal{V}$ is a Hilbert space if $\mathcal{V}$ with metric $d(v,w) := \|v-w\|$ is complete

Example 1.1 *Consider a measurable function* $]a,b[\ni x \mapsto \rho(x) > 0$. *(a can be* $-\infty$ *and b can be* $+\infty$*). We define* $L^2([a,b],\rho)$ *as the space of measurable functions*

$$f : [a,b] \to \mathbb{C}$$

such that

$$\int_a^b |f(x)|^2 \rho(x) \mathrm{d}x < \infty.$$

It is a Hilbert space if equipped with the scalar product

$$(f|g) := \int_a^b \overline{f(x)} g(x) \rho(x) \mathrm{d}x, \quad f, g \in L^2([a,b],\rho).$$

Example 1.2 *Let* $f_n(x) = n^\alpha x \mathrm{e}^{-nx}$ *and* $1 < \alpha < \frac{3}{2}$. *Then* $\sup f_n \to \infty$ *and* $\|f\|_2 \to 0$.

1.2 Orthogonal bases

Let $\mathcal{V}$ be a Hilbert space For $W \subset \mathcal{V}$, the orthogonal complement of W is

$$W^\perp := \{v \in \mathcal{V} \;:\; (w|v) = 0, \quad w \in W\}.$$

Note that $W^\perp$ is always a closed subspace of $\mathcal{V}$.

Let $\{f_1, f_2, \cdots\} \subset L^2([a,b],\rho)$. We say that it is an *orthogonal system* if

$$(f_n|f_m) = 0, \quad n \neq m.$$

If in addition $(f_n|f_n) = 1$, then we say that it is an *orthonormal system.*

We say that $\{f_1, f_2, \dots\}$ is an orthogonal basis in $\mathcal{V}$, if it is an orthogonal system, all its elements are nonzero, and $\{f_1, f_2, \dots\}^\perp = \{0\}$.

We say that $\{f_1, f_2, \dots\}$ is an orthonormal basis in $\mathcal{V}$ if it is an orthonormal system and $\{f_1, f_2, \dots\}^\perp = \{0\}$.

Obviously, if $\{f_1, f_2, \cdots\}$ is an orthogonal basis, then we can transform it into an orthonormal basis by replacing f_n with $\frac{f_n}{\|f_n\|}$.

Theorem 1.3 *Let $(f_1, f_2, \dots)$ be an orthonormal basis.*

(1) *Let $(c_1, c_2, \dots)$ be a complex sequence such that*

$$\sum_{j=1}^{\infty} |c_j|^2 < \infty. \tag{1.1}$$

Set

$$h_n := \sum_{j=1}^{n} c_j f_j. \tag{1.2}$$

Then there exists $h \in \mathcal{V}$ such that $\|h - h_n\| \to 0$.

(2) *Let $h \in \mathcal{V}$. Set $c_j := (f_j|h)$. Then (1.1) is true and if we define h_n as in (1.2), then $\|h - h_n\| \to 0$.*

Proof. (1) For $n \geq m$ we have

$$\|h_n - h_m\|^2 = \sum_{j=m+1}^{n} |c_j|^2. \tag{1.3}$$

From (1.1) we see that (1.3) converges to 0 when $n, m \to \infty$. Hence the sequence (h_n) is a Cauchy sequence. We know that the space $\mathcal{V}$ is complete. Therefore, (h_n) has a limit.

(2) First we check that

$$\sum_{j=1}^{n} |c_j|^2 \leq \|h\|^2.$$

Hence

$$\sum_{j=1}^{\infty} |c_j|^2 \leq \|h\|^2.$$

Therefore, (1.1) is satisfied. By (1) the limit $\tilde{h} := \lim_{n\to\infty} h_n$ exists. We check that $(h - \tilde{h}|f_j) = 0$, $j = 1, 2, \dots$. Hence $h - \tilde{h} = 0$. $\square$

We will write

$$\sum_{j=1}^{\infty} c_j f_j := h,$$

where h is defined as in the above theorem.

Example 1.4 *In* $L^2([-\pi,\pi])$, $e_n = \mathrm{e}^{\mathrm{i}n\phi}$, $n \in \mathbb{Z}$, *is an orthogonal basis and* $(e_n|e_n) = 2\pi$. *If* $f \in L^2([-\pi,\pi])$, *we obtain*

$$\left\| f - \lim_{n\to\infty} \frac{1}{2\pi} \sum_{|j|\leq n} \hat{f}_j \mathrm{e}^{\mathrm{i}n\phi} \right\| \to 0,$$

where

$$\hat{f}_n := \int_{-\pi}^{\pi} f(\phi)\mathrm{e}^{-\mathrm{i}n\phi}\mathrm{d}\phi$$

are Fourier coefficients *of* f.

Example 1.5 *Another related bases in* $L^2([-\pi,\pi])$ *are* $f_n^+ := \cos n\phi$, $f_n^- := \sin n\phi$, $n = 1,2,\dots$, $(f_n^\pm|f_n^\pm) = \pi$, $f_0 := 1$, $(f_0|f_0) = 2\pi$.

Example 1.6 *In* $L^2([0,\pi])$ *we have an orthogonal basis* $c_n := \cos n\phi$, $n = 1,2,\dots$, $(c_n|c_n) = \frac{\pi}{2}$, $c_0 = 1$, $(c_0|c_0) = \pi$. *Another orthogonal basis in* $L^2([0,\pi])$: $s_n := \sin n\phi$, $n = 1,2,\dots$, $(s_n|s_n) = \frac{\pi}{2}$.

There are functions, which have a more convenient expansions in cosines, other in sines:

$$\begin{aligned} 1 &= c_0 = \frac{1}{\pi}\sum_{m=0}^{\infty} \frac{2}{2m+1} s_{2m+1}, \\ \sin\phi &= s_1 = \frac{1}{\pi}\sum_{m=1}^{\infty} \Big(\frac{1}{2m-1} - \frac{1}{2m+1}\Big) c_{2m}. \end{aligned}$$

1.3 Fourier series

Example 1.7 $h(\phi) := (a - \mathrm{e}^{\mathrm{i}\phi})^{-1}$, $a > 1$. *Then*

$$\hat{h}_n = \begin{cases} 2\pi a^{-n-1}, & n = 0,1,\dots; \\ 0, & n = -1,-2,\dots. \end{cases}$$

Example 1.8 $h(\phi) := (\mathrm{e}^{\mathrm{i}\phi} - a)^{-1}$, $a < 1$. *Then*

$$\hat{h}_n = \begin{cases} 0, & n = 0,1,2,\dots; \\ 2\pi a^{-n-1}, & n = -1,-2,\dots. \end{cases}$$

Example 1.9 $h(\phi) := \phi$. *Then*

$$\hat{h}_n = \begin{cases} \frac{\mathrm{i}2\pi(-1)^n}{n}, & n \neq 0 \\ 0. & n = 0. \end{cases}$$

This follows from $h(\phi) = -\mathrm{i}\log(1+\mathrm{e}^{\mathrm{i}\phi}) + \mathrm{i}\log(1+\mathrm{e}^{-\mathrm{i}\phi})$.

If we sum up

$$h_{(n)}(\phi) := \sum_{|j|\leq n} \frac{\hat{h}_j \mathrm{e}^{\mathrm{i}n\phi}}{2\pi},$$

then we will notice in the neighborhood of $\phi = \pm\pi$ the so-called Gibbs phenomenon: the function $h_{(n)}$ “overshoots"' the functioni h. In fact,

$$h_{(n)}(-\pi + \epsilon) = -2\sum_{j=1}^{n} \frac{\sin \epsilon j}{j}.$$

In a neighborhood of discontinuities of h we notice "‘wiggles"' of $h_{(n)}$, which get narrower as n increases, but which does not reduce its height. This wiggle has a universal limiting shape. In fact

$$\lim_{n\to\infty} h_{(n)}\left(-\pi + \frac{c}{n}\right) = -2\int_0^c \frac{\sin x}{x}\mathrm{d}x.$$

Thus if a function has a discontinuity of the form of a jump $a\pi$, in the partial sum of the Fourier series there will be a jump $2ac$, where $c = \int_0^\pi \frac{\sin x}{x}\mathrm{d}x > \frac{\pi}{2}$ is the so-called *Wilbraham-Gibbs constant.*

1.4 Orthogonal projections

We say that an operator P is a projection if $P^2 = P$. A projection P is called orthogonal if $\mathrm{Ker}P = \mathrm{Ran}P^{\perp}$. Equivalently: $P = P^*$. We then say that P is the orthogonal projection onto $\mathrm{Ran}P$.

If v is a nonzero vector, then the orthogonal projection onto $\mathbb{C}v$ is

$$P_v w = \frac{v(v|w)}{(v|v)}.$$

In the physical literature this is often denoted as $\frac{|v)(v|}{(v|v)}$.

Ifi $v_1, \dots, v_n$ is an orthogonal basis of a subspace $\mathcal{V}_0$, then the orthogonal projection onto $\mathcal{V}_0$ is

$$P_{\mathcal{V}_0} = \sum_{j=1}^{n} \frac{|v_j)(v_j|}{(v_j|v_j)}.$$

Example 1.10 *Consider $L^2([-\pi,\pi])$. The orthogonal projection P_n onto the space spanned by $\mathrm{e}^{\mathrm{i}j\phi}$ z $|j| < n$ has the integral kernel*

$$P_n(\phi,\psi) = \frac{\sin\frac{(2n+1)(\phi-\psi)}{2}}{2\pi\sin\frac{(\phi-\psi)}{2}}.$$

Example 1.11 *Consider $L^2([0,\pi])$. The orthogonal projection P_n onto the space spanned by $\sin j\phi$, $j = 1, \dots, n$ has the integral kernel*

$$P_n(\phi,\psi) = \frac{\sin\frac{(2n+1)(\phi+\psi)}{2}}{2\pi\sin\frac{\phi+\psi}{2}} - \frac{\sin\frac{(2n+1)(\phi-\psi)}{2}}{2\pi\sin\frac{\phi-\psi}{2}}.$$

1.5 Gram-Schmidt orthogonalization

Let $(g_1, g_2, \dots)$ be a sequence of linearly independent vectors in the Hilbert space $\mathcal{V}$. Let $\mathcal{V}_n$ be the subspace spanned by $g_1, \dots, g_n$. Then $\mathcal{V}_n$ has dimansion n and $\mathcal{V}_1 \subset \mathcal{V}_2 \subset \cdots$.

We define inductively

$$f_n := g_n - \sum_{j=1}^{n-1} \frac{f_j (f_j | g_n)}{\|f_j\|^2} = (1 - P_{n-1}) g_n,$$

where P_n is the orthogonal projection onto $\mathcal{V}_n$. Then $(f_1, f_2, \dots)$ is an orthogonal system.

2 Orthogonal polynomials

2.1 Density of polynomials in a weighted space

Consider the space $L^2([a,b], \rho)$ defined in Example (1.1) Recall that

$$L^2([a,b], \rho) := \left\{ f : [a,b] \to \mathbb{C} \mid \int_a^b |f(x)|^2 \rho(x) \mathrm{d}x < \infty \right\}$$

with the scalar product

$$(f|g)_\rho := \int_a^b \overline{f(x)} g(x) \rho(x) \mathrm{d}x.$$

Suppose in addition that

$$\int_a^b |x|^n \rho(x) \mathrm{d}x < \infty, \quad n = 0, 1, \dots.$$

Then the monomials $1, x, x^2, \dots$ are a linearly independent system in $L^2([a,b], \rho)$. Applying the Gram-Schmidt construction we obtain orthogonal polynomials $P_0, P_1, P_2, \dots$. Note that $\mathrm{deg} P_n = n$.

There exists a simple criterion which allows us to check whether it is an orthogonal basis.

Theorem 2.1 *Suppose that for a certain $\epsilon > 0$*

$$\int_a^b \mathrm{e}^{\epsilon |x|} \rho(x) \mathrm{d}x < \infty.$$

Then polynomials are dense in $L^2([a,b], \rho)$. Hence, $P_0, P_1, \dots$ are an orthogonal basis of $L^2([a,b], \rho)$.

Proof. Let $h \in L^2([a,b], \rho)$. Then for $|\mathrm{Im} z| \leq \frac{\epsilon}{2}$

$$\int_a^b |\rho(x) h(x) \mathrm{e}^{-\mathrm{i}xz}| \mathrm{d}x \quad \leq \quad \left(\int_a^b \rho(x) \mathrm{e}^{\epsilon |x|} \mathrm{d}x \right)^{\frac{1}{2}} \left(\int_a^b \rho(x) |h(x)|^2 \mathrm{d}x \right)^{\frac{1}{2}} < \infty.$$

Hence for $|\mathrm{Im} z| \leq \frac{\epsilon}{2}$ we can define

$$F(z) := \int_a^b \rho(x) \mathrm{e}^{-\mathrm{i}zx} h(x) \mathrm{d}x.$$

Therefore, the function F is analytic in the strip $\{z \in \mathbb{C} \ : \ |\mathrm{Im} z| < \frac{\epsilon}{2}\}$. Let $(x^n|h) = 0$, $n = 0, 1, \ldots$. Then

$$\frac{\mathrm{d}^n}{\mathrm{d}z^n} F(z)\Big|_{z=0} = (-\mathrm{i})^n \int_a^b x^n \rho(x) h(x) \mathrm{d}x = (-\mathrm{i})^n (x^n|h) = 0.$$

But an analytic function which vanishes together with all its derivatives at one point is zero in the whole domain (if the domain is connected). Hence $F = 0$ in the whole strip, in particular on the real line. Thus $\hat{h} = 0$. Using the inverse Fourier transform we obtain $h = 0$.

Therefore, the orthogonal complement of the set of polynomials is zero. Hence polynomials are dense in $L^2([a, b], \rho)$. $\square$

2.2 Christoffel-Darboux formula

Let $P_0, P_1, P_2, \ldots$ be a basis of orthogonal polynomials Let $p_n(x) = \frac{P_n(x)}{\|P_n\|}$ be the corresponding orthonormal basis.

The matrix elements of the operator of multiplication by x are denoted

$$\beta_{jm} := (p_j|xp_m) = \int_a^b \rho(x) x p_j(x) p_m(x) \mathrm{d}x.$$

Let k_j be the coefficient of p_j at the power x^j.

Theorem 2.2

$$\beta_{jm} = \beta_{mj}, \tag{2.1}$$

$$\beta_{jm} = 0, \qquad |j - m| \geq 2, \tag{2.2}$$

$$\beta_{j,j+1} = \frac{k_j}{k_{j+1}}, \tag{2.3}$$

We have the recurrent formula

$$xp_n = \beta_{n,n-1} p_{n-1} + \beta_{n,n} p_n + \beta_{n,n+1} p_{n+1}. \tag{2.4}$$

Proof. (2.1) is obvious

Let us show (2.2). We can assume that $m + 2 \leq j$. Then xp_m is a polynomial of degree $m + 1 < j$. Hence it is orthogonal to p_j. Therefore, $(p_j|xp_m) = 0$.

We have

$$xp_j = k_j x^{j+1} + q = \frac{k_j}{k_{j+1}} p_{j+1} + r,$$

where $\deg q \leq j$ and $\deg r \leq j$. Hence

$$(xp_j|p_{j+1}) = \frac{k_j}{k_{j+1}}(p_{j+1}|p_{j+1}) + (r|p_{j+1}) = \frac{k_j}{k_{j+1}}.$$

(2.4) follows from

$$xp_n = \sum_{j=0}^{\infty} p_j(p_j|xp_n).$$

□

Theorem 2.3 (The Christoffel-Darboux formula) *The integral kernel of the orthogonal projection onto the space of polynomials of degree $\leq n$ is*

$$\begin{aligned} P_n(x,y) &= \sum_{k=0}^{n} p_k(x)p_k(y) \\ &= \tfrac{k_n}{k_{n+1}} \tfrac{p_n(y)p_{n+1}(x) - p_{n+1}(y)p_n(x)}{x-y}, \end{aligned}$$

and on the diagonal

$$P_n(x,x) = \frac{k_n}{k_{n+1}}(p_n(x)p'_{n+1}(x) - p_{n+1}(x)p'_n(x)).$$

Proof. Let Q_k be the orthogonal projection onto p_k. Its integral kernel is

$$Q_k(x,y) = p_k(x)p_k(y).$$

The integral kernel of $[x, Q_k]$ is

$$\begin{aligned} xQ_k(x,y) - Q_k(x,y)y &= xp_k(x)p_k(y) - p_k(x)p_k(y)y \\ &= \beta_{k,k-1}(p_{k-1}(x)p_k(y) - p_k(x)p_{k-1}(y)) \\ &\quad + \beta_{k+1,k}(p_{k+1}(x)p_k(y) - p_k(x)p_{k+1}(y)). \end{aligned}$$

Hence, $[x, P_n] = \sum_{k=0}^{n}[x, Q_k]$ has the integral kernel

$$xP_n(x,y) - P_n(x,y)y = \beta_{n,n+1}(p_{n+1}(x)p_n(y) - p_n(x)p_{n+1}(y)).$$

□

2.3 Chebyshev polynomials of the 1st kind

Consider the space

$$L^2([-1,1],(1-x^2)^{-\frac{1}{2}}).$$

Define

$$\begin{aligned} T_n(\cos\phi) &= \cos n\phi, & \phi \in [0,\pi], \\ T_n(x) &= \tfrac{1}{2}((x + \mathrm{i}\sqrt{1-x^2})^n + (x - \mathrm{i}\sqrt{1-x^2})^n), & x \in [-1,1]. \end{aligned}$$

Theorem 2.4 *The polynomials T_m form an orthogonal basis such that*

$$\|T_0\|^2 = \pi, \qquad \|T_n\|^2 = \frac{\pi}{2}, \quad n = 1, 2, \dots .$$

They satisfy the equation

$$((1 - x^2)\partial_x^2 - x\partial_x + n^2)T_n(x) = 0. \tag{2.5}$$

Proof. Define

$$\begin{aligned} W : L^2([-1,1], (1-x^2)^{-\frac{1}{2}}) &\to L^2([0,\pi]), \\ Wf(\phi) &:= f(\cos\phi). \end{aligned}$$

Then

$$\|Wf\|^2 = \int_0^\pi |f(\cos\phi)|^2 \mathrm{d}\phi = -\int_0^\pi |f(\cos\phi)|^2 \sin^{-1}\phi \mathrm{d}\cos\phi = \int_{-1}^1 |f(x)|^2 (1-x^2)^{-\frac{1}{2}} \mathrm{d}x.$$

Hence W is a unitary operator. Besides,

$$WT_n(\phi) = T_n(\cos\phi) = \cos n\phi.$$

We have

$$(\partial_\phi^2 + n^2)\cos n\phi = 0. \tag{2.6}$$

To see (2.5), we compute:

$$\partial_\phi Wf(\phi) = -\sin\phi f'(\cos\phi),$$

$$W^*\partial_\phi Wf(x) = -\sin(\arccos x) f'(x) = -(1-x^2)^{\frac{1}{2}}\partial_x f(x).$$

Hence

$$\begin{aligned} W^*\partial_\phi W &= -(1-x^2)^{\frac{1}{2}}\partial_x, \\ W^*\partial_\phi^2 W = (W^*\partial_\phi W)^2 &= (1-x^2)\partial_x^2 - x\partial_x. \end{aligned}$$

□

Properties:

$$\begin{aligned} |T_n(x)| &\leq 1, \quad |x| < 1, \\ T_n(\pm 1) &= (\pm 1)^n, \\ \sum_{n=0}^\infty T_n(x) r^n &= \frac{1 - rx}{1 - 2rx + r^2}, \\ \sum_{n=1}^\infty T_n(x) \frac{r^n}{n} &= -\log(1 - 2rx + r^2). \end{aligned}$$

2.4 Chebyshev polynomials of the 2nd kind

Consider the space

$$L^2([-1,1],(1-x^2)^{\frac{1}{2}}).$$

Define

$$\begin{aligned} U_n(\cos\phi) &= \frac{\sin(n+1)\phi}{\sin\phi}, & \phi\in[0,\pi], \\ U_n(x) &= \frac{(x+\mathrm{i}\sqrt{1-x^2})^{n+1}-(x-\mathrm{i}\sqrt{1-x^2})^{n+1}}{2\mathrm{i}\sqrt{1-x^2}}, & x\in[-1,1]. \end{aligned}$$

Theorem 2.5 *The polynomials U_m are an orthogonal basis and*

$$\|U_n\|^2=\frac{\pi}{2},\quad n=0,1,2,\dots.$$

The satisfy the equation

$$((1-x^2)\partial_x^2-3x\partial_x+n(n+2))U_n(x)=0. \tag{2.7}$$

Proof. Define

$$\begin{aligned} V:L^2([-1,1],(1-x^2)^{\frac{1}{2}})&\to L^2([0,\pi]), \\ Vf(\phi)&:=f(\cos\phi)\sin\phi. \end{aligned}$$

Then

$$\|Vf\|^2=\int_0^\pi|f(\cos\phi)|^2\sin^2\phi\mathrm{d}\phi=-\int_0^\pi|f^2(\cos\phi)|\sin\phi\mathrm{d}\cos\phi=\int_{-1}^1|f(x)|^2(1-x^2)^{\frac{1}{2}}\mathrm{d}x.$$

Hence the operator V is unitary. Besides,

$$VU_n(\phi)=U_n(\cos\phi)\sin\phi=\sin(n+1)\phi.$$

We have

$$(\partial_\phi^2+(n+1)^2))\sin(n+1)\phi=0. \tag{2.8}$$

To see (2.7), we compute:

$$\partial_\phi Vf(\phi)=-\sin^2\phi f'(\cos\phi)+\cos\phi f(\cos\phi),$$

Hence,

$$\begin{aligned} V^*\partial_\phi V&=-(1-x^2)^{\frac{1}{2}}\partial_x+x(1-x^2)^{-\frac{1}{2}}, \\ [V^*\partial_\phi^2V=(V^*\partial_\phi V)^2&=(1-x^2)\partial_x^2-3x\partial_x-1. \end{aligned}$$

□

Properties:

$$\begin{aligned} |U_n(x)| &\le (1-x^2)^{-1/2},\quad |x|<1, \\ U_n(\pm1) &= (\pm1)^n(n+1), \\ \sum_{n=0}^\infty U_n(x)r^n &= (1-2rx+r^2)^{-1}. \end{aligned}$$

3 Operators

3.1 Bounded operators

Let A be a linear operator from a Hilbert space $\mathcal{V}$ into $\mathcal{W}$. We say that A is bounded if

$$\sup\{\|Av\| \ : \ v \in \mathcal{V},\ \|v\| \leq 1\} =: \|A\|$$

is finite. The set of bounded operators from $\mathcal{V}$ into $\mathcal{W}$ is denoted $B(\mathcal{V}, \mathcal{W})$. Ifi $\mathcal{V} = \mathcal{W}$, we write $B(\mathcal{V}) = B(\mathcal{V}, \mathcal{V})$.

3.2 Integral kernel

Consider the space $L^2([a,b],\rho)$. Often an operator A on $L^2([a,b],\rho)$ can be described by a function $[a,b] \times [a,b] \ni (x,y) \mapsto A(x,y)$ such that

$$Af(x) := \int_a^b A(x,y) f(y) \rho(y) \mathrm{d}y.$$

For instance, if $v_1, \dots, v_n$ is an orthonormalbasis of a subspace $\mathcal{V}_0$, then $P_{\mathcal{V}_0}$, hence the orthogonal projection onto $\mathcal{V}$, has the integral kernel

$$P_{\mathcal{V}_0}(x,y) = \sum_{j=1}^{n} v_j(x) \overline{v_j(y)}.$$

We can show that if $\int_a^b |A(x,y)|^2 \rho(x) \mathrm{d}x \rho(y) \mathrm{d}y < \infty$, then A is a bounded operator.

3.3 Adjoint operators

Let $A \in B(\mathcal{V}, \mathcal{W})$. Then

$$(w|Av) = (A^* w|v), \quad v \in \mathcal{V},\ w \in \mathcal{W}$$

defines the operator A^* (Hermitian) conjugate to A. We have $A^* \in B(\mathcal{W}, \mathcal{V})$. If the integral kernel of A is $A(x,y)$, then the integral kernel of A^* is $\overline{A}(y,x)$.

We say that A is self-adjoint if

$$A = A^*.$$

We say that A is unitary if

$$AA^* = A^* A = 1.$$

A is normal if

$$AA^* = A^* A.$$

3.4 Point spectrum

Let A be a linear operator on a vector space $\mathcal{V}$. Recall that $\lambda \in \mathbb{C}$ is an eigenvalue of A if there exists a nonzero vector $v \in \mathcal{V}$ such that $Av = \lambda v$. The set of eigenvalues of A is called the point spectrum of A and is denoted by $\mathrm{sp_p}(A)$.

3.5 Spectrum

Assume in addition that $\mathcal{V}$ is a Hilbert space and B a bounded operator on $\mathcal{V}$.. We say that B is invertible if B is a bijection and B^{-1} is bounded.

We say that $\lambda \in \mathbb{C}$ belongs to the spectrum of A if $\lambda - A$ is not invertible. The spectrum of A is denoted $\mathrm{sp}(A)$.

If $z \in \mathbb{C}$ does not belong to $\mathrm{sp}A$, then there exists the resolvent of the operator A

$$(z - A)^{-1}.$$

It is easy to see that the point spectrum of A is a subset of its spectrum, that is, $\mathrm{sp_p}(A) \subset \mathrm{sp}(A)$. In fact, let $v \in \mathrm{sp_p}(A)$, or $Av = \lambda v$, $v \neq 0$. Then $(\lambda - A)v = 0$, hence $\lambda - A$ is not injective, so that $\lambda \in \mathrm{sp}(A)$.

3.6 Spectrum in finite dimension

Assume that the space $\mathcal{V}$ is finite dimensional. Then there exist convenient criteria for the invertibility of linear operators.

Theorem 3.1 *Let B be an operator on $\mathcal{V}$. Then the following conditions are equivalent:*

(1) *B is invertible*

(2) $\mathrm{Ker}B = \{0\}$.

(3) $\det B \neq 0$

Therefore, in finite dimension the spectrum can be determined by several methoids:

Theorem 3.2 *Let A be anoperator on $\mathcal{V}$ and $\lambda \in \mathbb{C}$. Then the following conditions are equivalent:*

(1) *λ is an eigenvalue of A.*

(2) *$\lambda - A$ is not invertible*

(3) $\det(\lambda - A) = 0$.

In infinite dimension the first condition implies the second, but the third condition usually is meaningless.

3.7 Spectral Theorem in finite dimension

Spectral Theorem in finite dimension belongs to the basic linear algebra course:

Theorem 3.3 *Let A be a normal operator on a finite dimensional Hilbert space. Then there exists an orthonormal basis of eigenvectors of A.*

A is self-adjoint iff all its eigenvalues are real.

A is unitary iff its all eigenvectors have absolute value 1.

Example 3.4 *Let e_j, $j = 1, \dots, n$, be the canonical basis of $\mathbb{C}^n$. Define the operator U by*

$$Ue_j := e_{j+1}, \quad j = 1, \dots, n-1, \quad Ue_n = e_1.$$

Then U is unitary, its eigenvalues are $\mathrm{e}^{\frac{\mathrm{i}k2\pi}{n}}$, $k = 0, \dots, n-1$ with corresponding normed eigenvectors

$$w_k = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \mathrm{e}^{\frac{\mathrm{i}jk2\pi}{n}} e_j.$$

Example 3.5 *Let $v\sigma = \sum_{i=1}^{3} v_i \sigma_i$, where $v_1, v_2, v_3 \in \mathbb{R}$ and σ_i are the Pauli matrices on $\mathbb{C}^2$. Then $v\sigma$ is self-adjoint. It is unitary if $v_1^2 + v_2^2 + v_3^2 = 1$. Eigenvalues are $\pm\sqrt{v_1^2 + v_2^2 + v_3^2}$ and eigenvectors*

$$w_+ = \sqrt{1+v_1}e_1 + \frac{v_2 + v_3}{\sqrt{1+v_1}} e_2, \quad w_- = \sqrt{1-v_1}e_1 + \frac{-v_2 + v_3}{\sqrt{1-v_1}} e_2.$$

3.8 Continuous spectrum

In an infinite dimensional Hilbert space one can formulate a generalization of Spectral Theorem. It is however more difficult. Below we discuss the first additional difficulty, which appears in infinite dimension.

Eigenvectors corresponding to distinct eigenvalues are orthogonal to one another. There may be a *continuous spectrum.*

Example 3.6 *On $L^2([0,1])$ we define $(Af)(x) = xf(x)$. This operator is self-adjoint, but has no eigenvectors.*

Example 3.7 *On $L^2(\mathbb{Z})$, let e_j denote the canonical basis. Define the operator U by $Ue_n := e_{n+1}$. It is unitary, but has no eigenvectors.*

3.9 Unbounded operators

One of the most inconvenient aspects of the operator theory on infinitely dimensional spaces, is the unboundedness of many physicaly important operators. This is related to an additional trouble: in practice such operators are not defined on the whole Hilbert space, only on its dense subspace. This subspace is called the domain of a given operator. The domain of the operator A will be denoted $\mathrm{Dom}A$.

This problem is absent in finite dimensions, where all operators are bounded.

Example 3.8 *On $L^2(\mathbb{R})$, let us try to define the operator $(Af)(x) = xf(x)$. The vector $(x+\mathrm{i})^{-1}$ belongs to $L^2(\mathbb{R})$, but $x(x+\mathrm{i})^{-1}$ does not belong to $L^2(\mathbb{R})$. Thus $(x+\mathrm{i})^{-1}$ does not belong to the domain of A.*

Example 3.9 *On $L^2(\mathbb{R})$ let us try to define the operator $pf(x) = \frac{1}{\mathrm{i}}\partial_x f(x)$. The vector $\theta(x)\mathrm{e}^{-x}$ belongs to $L^2(\mathbb{R})$, but $\frac{1}{\mathrm{i}}\partial_x \theta(x)\mathrm{e}^{-x}$ does not belong to $L^2(\mathbb{R})$. ($\theta(x)$ denotes the Heaviside function). Therefore, $\theta(x)\mathrm{e}^{-x}$ does not belong to the domain of p.*

3.10 Spectrum of unbounded operators

Let A be a linear operator, perhaps unbounded, with domain $\mathrm{Dom}(A) \subset \mathcal{V}$.

$\lambda \in \mathbb{C}$ is an eigenvalue of A if there exists $v \in \mathrm{Dom}(A)$ such that $Av = \lambda v$. The set of eigenvalues is called the *point spectrum* of A. It is denoted by $\mathrm{sp_p}(A)$.

We say that A is *invertible* if it is a bijection $\mathrm{Dom}(A) \to \mathcal{V}$ and A^{-1} (which is defined on the whole $\mathcal{V}$) is bounded.

We say that $\lambda \in \mathbb{C}$ belongs to the spectrum of A, if $\lambda - A$ is not invertible. The spectrum of A is denoted by $\mathrm{sp}(A)$.

In the same way as for bounded operators we show that $\mathrm{sp_p}(A) \subset \mathrm{sp}(A)$.

3.11 Hermiticity

For unbounded operators there exist more than one generalization of the concept of self-adjointness (Hermiticity).

Consider a Hilbert space $\mathcal{V}$. Let A be an operator with domain $\mathrm{Dom}A$, which is a dense subspace of $\mathcal{V}$. Let the image of A be in $\mathcal{V}$. We say that A is Hermitian (or symmetric) if

$$(w|Av) = (Aw|v), \quad v, w \in \mathrm{Dom}A.$$

This is a condition which is easy to check in practice. Unfortunately, from the theoretical point of view the more interesting concepts are the self-adjointness and essential self-adjointness, which are more difficult to formulate. Every self-adjoint operator is essentially self-adjoint. Every essentially self-adjoint operator is Hermitian. However, the converse statements are in general not true.

The Hermiticity itself is enough to show the following properties:

Theorem 3.10 *Let A be a Hermitian operator with domain* $\mathrm{Dom}A$.

(1) *If $v \in \mathrm{Dom}A$ is an eigenvector with eigenvalue λ, that is $Av = \lambda v$, then $\lambda \in \mathbb{R}$.*

(2) *If $\lambda_1 \neq \lambda_2$ eigenvalues with eigenvectors v_1 and v_2, then v_1 is orthogonal to v_2.*

Proof. The proof is identical as in the finite dimensional case. To prove (1) we compute:

$$\lambda(v|v) = (v|Av) = (Av|v) = \overline{\lambda}(v|v).$$

Then we divide by $(v|v) \neq 0$.

Proof of (2):

$$(\lambda_1 - \lambda_2)(v_1|v_2) = (Av_1|v_2) - (v_1|Av_2) = (v_1|Av_2) - (v_1|Av_2) = 0.$$

□

3.12 Self-adjointness and essential self-adjointness

The material of this subsection will not be used in what follows.

Let A be an operator with domain $\mathrm{Dom}(A)$ dense in $\mathcal{V}$. The operator A^* is defined as follows: We say that $w \in \mathrm{Dom}(A^*)$ iff there exists $u \in \mathcal{V}$ such that

$$(w|Av) = (u|v), \quad v \in \mathrm{Dom}(A).$$

Using the density of $\mathrm{Dom}(A)$ we see that such a $u \in \mathcal{V}$ is defined uniquely. We then set $A^*w := u$.

We say that

$$A \text{ is } \textit{self-adjoint}, \text{ if} \qquad A = A^*; \tag{3.1}$$

$$\text{A is } \textit{essentially self-adjoint}, \text{ if} \qquad A^{**} = A^*. \tag{3.2}$$

We have implications

$$A \text{ is self-adjoint} \Rightarrow A \text{ is essentially self-adjoint} \Rightarrow A \text{ is Hermitian.}$$

The best property is the self-adjointness. The Spectral Theorem can be generalized to infinite dimension for self-adjoint operators.

Essntially self-adjoint operators extend uniquely to self-adjoint ones, hence this is also a good property.

Hermitian operators can be somewhat bizarre. In practice, it may be non-trivial to check the self-adjointness of a Hermitian operator.

4 Differential operators

Differential operators is an especially important class of operators. Unfortunately, they are unbounded, and it can be quite nontrivial to check whether they are self-adjoint. This is related to the so-called boundary conditions. Let us first discuss this in simple examples.

4.1 The momentum operator on an interval

Consider the operator $pf(x) = \frac{1}{\mathrm{i}}\partial_x f(x)$ defined on the domain $f \in C^\infty([-\pi, \pi])$ treated as a subspace of the Hilbert space $L^2([-\pi, \pi]$. Suppose we want to find its eigenvalues, that is, we solve the equation

$$\frac{1}{\mathrm{i}}\partial_x f = \lambda f, \quad f \in C^\infty([-\pi, \pi]). \tag{4.1}$$

Clearly, this equation is solved by $f(x) = c\mathrm{e}^{\mathrm{i}\lambda x}$ for any $\lambda \in \mathbb{C}$. This means we have many solutions, which indicates that this equation (and the operator p) is not very useful in applications.

Let us modify the problem by reducing the domain. Let us restrict ourselves to $f \in C^\infty([-\pi, \pi])$ that satisfy the boundary conditions

$$f(\pi) = \mathrm{e}^{\mathrm{i}2\pi\kappa} f(-\pi).$$

The operator $\frac{1}{\mathrm{i}}\partial_x$ with this domain will be denoted p_κ. (4.1) then has solutions $\lambda = n+\kappa$, wher $n\in\mathbb{Z}$, and eigenfunctions $e_n(x) = \mathrm{e}^{\mathrm{i}(\kappa+n)x}$. The eigenfunctions form an orthogonal basis in $L^2([-\pi,\pi])$. The operator p has spectrum $\mathrm{sp}p_\kappa = \mathrm{sp_p}p = \{n+\kappa \ : \ n\in\mathbb{Z}\}$.

The operator p_κ is Hermitian (and even essentially self-adjoint). It is a useful operator, useful in applications. The Hermiticity condition is easy to check by integration by parts:

$$\begin{aligned}(f|p_\kappa g) &= \int_{-\pi}^{\pi}\overline{f(x)}\frac{1}{\mathrm{i}}\partial_x g(x)\mathrm{d}x \\ &= \int_{-\pi}^{\pi}\left(\overline{\frac{1}{\mathrm{i}}\partial_x f(x)}\right)g(x)\mathrm{d}x + \frac{1}{\mathrm{i}}\left(\overline{f(\pi)}g(\pi)-\overline{f(-\pi)}g(-\pi)\right) = (p_\kappa f|g),\end{aligned}$$

where the boundary terms vanish by biundary conditions.

Let us compute the resolvent of p_κ, that is $R_\kappa(z) = (z-p_\kappa)^{-1}$. Let $(z-p_\kappa)g = f$, or

$$(z-\frac{1}{\mathrm{i}}\partial_x)g(x) = f(x). \tag{4.2}$$

The homogenous equation

$$(z-\frac{1}{\mathrm{i}}\partial_x)g(x) = 0. \tag{4.3}$$

is solved by $g(x) = \mathrm{e}^{\mathrm{i}zx}$. We use the variation of the constant method: $g(x) = c(x)\mathrm{e}^{\mathrm{i}zx}$. We obtain

$$\mathrm{i}c'(x)\mathrm{e}^{\mathrm{i}zx} = f(x)$$

Hence,

$$\begin{aligned}c(x) &= c(-\pi) - \mathrm{i}\int_{-\pi}^{x}\mathrm{e}^{\mathrm{i}zy}f(y)\mathrm{d}y \\ &= c(\pi) + \mathrm{i}\int_{x}^{\pi}\mathrm{e}^{\mathrm{i}zy}f(y)\mathrm{d}y.\end{aligned}$$

g belongs to the domain of p_κ when $g(\pi) = \mathrm{e}^{\mathrm{i}2\pi\kappa}g(-\pi)$, which yields

$$c(\pi) = \mathrm{e}^{\mathrm{i}2\pi(\kappa-z)}c(-\pi).$$

Therefore,

$$\begin{aligned}\mathrm{i}\int_{-\pi}^{\pi}\mathrm{e}^{-\mathrm{i}zy}f(y)\mathrm{d}y &= c(-\pi)-c(\pi) \\ &= c(-\pi)(1-\mathrm{e}^{\mathrm{i}2\pi(\kappa-z)}).\end{aligned}$$

Hence,

$$\begin{aligned}c(-\pi) &= \frac{\mathrm{i}}{1-\mathrm{e}^{\mathrm{i}2\pi(\kappa-z)}}\int_{-\pi}^{\pi}\mathrm{e}^{-\mathrm{i}zy}f(y), \\ g(x) &= \frac{\mathrm{i}}{1-\mathrm{e}^{-\mathrm{i}2\pi(\kappa-z)}}\int_{-\pi}^{x}\mathrm{e}^{\mathrm{i}z(x-y)}f(y)\mathrm{d}y \\ &\quad + \frac{\mathrm{i}}{1-\mathrm{e}^{\mathrm{i}2\pi(\kappa-z)}}\int_{x}^{\pi}\mathrm{e}^{\mathrm{i}z(x-y)}f(y)\mathrm{d}y.\end{aligned}$$

Therefore, the integral kernel of $R_\kappa(z) = (z - p_\kappa)^{-1}$ (called sometimes Green's function) is

$$\begin{aligned} R_\kappa(z)(x,y) &= \frac{\mathrm{i}}{1 - \mathrm{e}^{-\mathrm{i}2\pi(\kappa - z)}} \mathrm{e}^{\mathrm{i}z(x-y)}\theta(x-y) \\ &\quad + \frac{\mathrm{i}}{1 - \mathrm{e}^{\mathrm{i}2\pi(\kappa - z)}} \mathrm{e}^{\mathrm{i}z(x-y)}\theta(y-x). \end{aligned}$$

For $z \in \mathbb{Z} + \kappa$, the resolvent $R_\kappa(z)$ is not defined, for remaining z it is a bounded operator.

4.2 Laplacian on an interval

Consider the space $L^2([0,\pi])$. Let $\mathcal{D}_{\min}$ be the set of functions $f \in C^\infty([0,\pi])$ equal zero on a neighborhood of 0 and π. It is a dense subspace of $L^2([0,\pi])$.

Define the operator on $\mathcal{D}_{\min}$ by the formula

$$H_{\min} f := -\partial_x^2 f(x), \quad f \in \mathcal{D}_{\min}.$$

Note that it does not possess eigenvectors. It satisfies the Hermiticity condition, which follows by integration by parts:

$$\begin{aligned} (g|H_{\min} f) &= -\int_0^\pi \overline{g}(x)\partial_x^2 f(x)\mathrm{d}x \\ &= -\int_0^\pi (\partial_x^2 \overline{g}(x)) f(x)\mathrm{d}x = (H_{\min} g|f). \end{aligned} \tag{4.4}$$

The operator $H_{\min}$ is not very interesting, because its domain is too small.

Replace now $\mathcal{D}_{\min}$ with $\mathcal{D}_{\max}$ consisting of all smooth functions on $[0,\pi]$. The operator $H_{\max}$ is defined with the same formula as $H_{\min}$, the only difference is that it has the domain $\mathcal{D}_{\max}$:

$$H_{\max} f := -\partial_x^2 f(x), \quad f \in \mathcal{D}_{\max}.$$

All complex numbers are eigenvalues of $H_{\max}$, because $f_\omega(x) = \mathrm{e}^{\mathrm{i}\omega x}$ satisfies

$$H_{\max} f_\omega = \omega^2 f_\omega. \tag{4.5}$$

Eigenvectors belonging to distinct eigenvalues are usually not mutually orthogonal. The operator $H_{\max}$ is not Hermitian, because when we integrate by parts boundary terms appear:

$$\begin{aligned} (g|H_{\max} f) &= -\int_0^\pi \overline{g}(x)\partial_x^2 f(x)\mathrm{d}x \qquad (4.6) \\ &= \overline{g}(0)\partial_x f(0) - \overline{g}(\pi)\partial_x f(\pi) + \int_0^\pi (\partial_x \overline{g}(x))\partial_x f(x)\mathrm{d}x \\ &= \overline{g}(0)\partial_x f(0) - \overline{g}(\pi)\partial_x f(\pi) - (\partial_x \overline{g}(0)) f(0) + (\partial_x \overline{g}(\pi)) f(\pi) - \int_0^\pi (\partial_x^2 \overline{g}(x)) f(x)\mathrm{d}x \\ &= \overline{g}(0)\partial_x f(0) - \overline{g}(\pi)\partial_x f(\pi) - (\partial_x \overline{g}(0)) f(0) + (\partial_x \overline{g}(\pi)) f(\pi) + (H_{\max} g|f). \end{aligned}$$

This means that $H_{\max}$ is not very interesting, because its domain is too large.

4.3 Laplacian on an interval with Dirichleta boundary conditions

Let H_D be equal $-\partial_x^2$ on smooth functions satisfying $f(0) = f(\pi) = 0$. Then the operator H_D defines a self-adjoint operator called the Laplacian with the Dirichlet boundary conditions. Its eigenvectors can be organized in an orthonormal basis:

$$s_n(x) = \sqrt{\frac{2}{\pi}} \sin xn, \quad H_\mathrm{D} s_n = n^2 s_n, \quad n = 1, 2, \dots. \tag{4.7}$$

Hence

$$\mathrm{sp} H_\mathrm{D} = \mathrm{sp}_\mathrm{p} H_\mathrm{D} = \{n^2 \ : \ n = 1, 2, \dots\}.$$

We can compute its resolvent $R_\mathrm{D}(\omega^2) = (\omega^2 - H_\mathrm{D})^{-1}$. Let

$$(\partial_x^2 + \omega^2) g(x) = f(x), \quad g(0) = g(\pi) = 0.$$

We use the variation of the constant method: $c_+(\pi) = c_-(0) = 0$,

$$\begin{aligned} g(x) &= c_+(x) \sin \omega x + c_-(x) \sin \omega(x - \pi), \\ g'(x) &= c_+(x) \omega \cos \omega x + c_-(x) \omega \cos \omega(x - \pi). \end{aligned}$$

Hence , assuming that $\sin \omega \neq 0$, we obtain

$$\begin{aligned} c_+'(x) \sin \omega x + c_-'(x) \sin \omega(x - \pi) &= 0, \\ c_+'(x) \omega \cos \omega x + c_-'(x) \omega \cos \omega(x - \pi) &= f(x); \end{aligned}$$

$$\begin{aligned} -c_+'(x) &= f(x) \frac{\sin \omega(x - \pi)}{\omega \sin \omega\pi}, \\ c_-'(x) &= f(x) \frac{\sin \omega x}{\omega \sin \omega\pi}; \end{aligned}$$

$$\begin{aligned} c_+(x) &= \int_x^\pi \frac{\sin \omega(y - \pi)}{\omega \sin \omega\pi} f(y) \mathrm{d}y, \\ c_-(x) &= \int_0^x \frac{\sin \omega y}{\omega \sin \omega\pi} f(y) \mathrm{d}y; \end{aligned}$$

$$\begin{aligned} g(x) &= \sin \omega x \int_x^\pi \frac{\sin \omega(y - \pi)}{\omega \sin \omega\pi} f(y) \mathrm{d}y \\ &\quad + \sin \omega(x - \pi) \int_0^x \frac{\sin \omega y}{\omega \sin \omega\pi} f(y) \mathrm{d}y. \end{aligned}$$

Therefore, the integral kernel of the resolvent $R_\mathrm{D}(\omega)$ (also called Green's function for the DIrichlet problem) is

$$\begin{aligned} R_\mathrm{D}(\omega^2)(x, y) &= \frac{\sin \omega x \sin \omega(y - \pi) \theta(y - x)}{\omega \sin \omega\pi} \\ &\quad + \frac{\sin \omega(x - \pi) \sin \omega y \theta(x - y)}{\omega \sin \omega\pi} \end{aligned}$$

It can be also computed by a different method:

$$R_\mathrm{D}(\omega^2)(x, y) = \sum_{n=1}^\infty \frac{2 \sin(xn) \sin(yn)}{\pi(\omega^2 - n^2)}. \tag{4.8}$$

4.4 Laplacian on an interval with Neumanna boundary conditions

Let $H_{\rm N}$ equal $-\partial_x^2$ on smooth functions satisfying $f'(0) = f'(\pi) = 0$. $H_{\rm N}$ defines the Laplacian with Neumann boundary conditions. Its eigenvectors form an orthonormal basis

$$c_0 := \frac{1}{\sqrt{\pi}}, \quad c_n(x) = \sqrt{\frac{2}{\pi}}\cos xn, \quad H_{\rm N}c_n = n^2 c_n, \quad n = 1, 2, \dots. \tag{4.9}$$

Hence

$$\mathrm{sp}H_{\rm N} = \mathrm{sp_p}H_{\rm N} = \{n^2 \ : \ n = 0, 1, 2, \dots\}.$$

Here is its resolvent: $R_{\rm N}(\omega^2) = (\omega^2 - H_{\rm N})^{-1}$. Let

$$(\partial_x^2 + \omega^2)g(x) = f(x), \quad g'(0) = g'(\pi) = 0.$$

By variation of the constant:: $c_+(\pi) = c_-(0) = 0$,

$$\begin{aligned} g(x) &= c_+(x)\cos\omega x + c_-(x)\cos\omega(x-\pi), \\ g'(x) &= -c_+(x)\omega\sin\omega x - c_-(x)\omega\sin\omega(x-\pi). \end{aligned}$$

Hence

$$\begin{aligned} c_+'(x)\cos\omega x + c_-'(x)\cos\omega(x-\pi) &= 0, \\ -c_+'(x)\omega\sin\omega x - c_-'(x)\omega\sin\omega(x-\pi) &= f(x); \end{aligned}$$

$$\begin{aligned} -c_+'(x) &= f(x)\frac{\cos\omega(x-\pi)}{\omega\sin\omega\pi}, \\ c_-'(x) &= f(x)\frac{\cos\omega x}{\omega\sin\omega\pi}; \end{aligned}$$

$$\begin{aligned} c_+(x) &= \int_x^\pi \frac{\cos\omega(y-\pi)}{\omega\sin\omega\pi}f(y)\mathrm{d}y, \\ c_-(x) &= \int_0^x \frac{\cos\omega y}{\omega\sin\omega\pi}f(y)\mathrm{d}y; \end{aligned}$$

$$\begin{aligned} g(x) &= \cos\omega x\int_x^\pi \frac{\cos\omega(y-\pi)}{\omega\sin\omega\pi}f(y)\mathrm{d}y \\ &\quad + \sin\omega(x-\pi)\int_0^x \frac{\cos\omega y}{\omega\sin\omega\pi}f(y)\mathrm{d}y. \end{aligned}$$

Thus the integral kernel of the resolvent $R_{\rm N}(\omega)$ (Green's function for the Neumann boundary conditions) is

$$\begin{aligned} R_{\rm N}(\omega^2)(x,y) &= \frac{\cos\omega x\cos\omega(y-\pi)\theta(y-x)}{\omega\sin\omega\pi} \\ &\quad + \frac{\cos\omega(x-\pi)\cos\omega y\theta(x-y)}{\omega\sin\omega\pi}. \end{aligned}$$

The resolvent can be computed by another method:

$$R_{\rm N}(\omega^2)(x,y) = \frac{1}{\pi\omega^2} + \sum_{n=1}^\infty \frac{2\cos(xn)\cos(yn)}{\pi(\omega^2 - n^2)}. \tag{4.10}$$

4.5 Laplacian with periodic boundary conditions

Let H_{per} be $-\partial_x^2$ on smooth functions satisfying $f(0) = f(\pi)$, $f'(0) = f'(\pi)$. H_{per} defines the Laplacian with periodic boundary conditions. Here is an orthonormal basis made of its eigenvectors:

$$e_n(x) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{\mathrm{i}2nx}, \quad H_{\mathrm{per}}e_n = 4n^2 e_n, \quad n = 0, \pm 1, \pm 2, \dots. \tag{4.11}$$

Hence

$$\mathrm{sp}H_{\mathrm{per}} = \mathrm{sp}_{\mathrm{p}}H_{\mathrm{per}} = \{4n^2 \ : \ n = 0, 1, 2, \dots\}.$$

Note that its eignevalues corresponding to $n = 1, 2, \dots$ are doubly degenerate.

4.6 Laplacian with antiperiodic boundary conditions

Let H_{per} be $-\partial_x^2$ on smooth functions satisfying $f(0) = -f(\pi)$, $f'(0) = -f'(\pi)$. H_{ant} defines the Laplacian with antiperiodic boundary conditions. Here is an orthonormal basis made of its eigenvectors:

$$f_n(x) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{\mathrm{i}(2n+1)x}, \quad H_{\mathrm{per}}e_n = (2n+1)^2 e_n, \quad n \in \mathbb{Z}. \tag{4.12}$$

Hence

$$\mathrm{sp}H_{\mathrm{per}} = \mathrm{sp}_{\mathrm{p}}H_{\mathrm{per}} = \{(2n+1)^2 \ : \ n = 0, 1, 2, \dots\}.$$

and all its eignevalues are doubly degenerate.

4.7 Some series

Proposition 4.1

$$\sum_{n=-\infty}^{\infty} \frac{1}{(n-\alpha)^2 - \omega^2} = \frac{\pi \sin(2\omega\pi)}{2\omega \sin(\alpha - \omega)\pi \sin(\alpha + \omega)\pi}, \tag{4.13}$$

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 - \omega^2} = -\frac{\pi \cos(\omega\pi)}{\omega \sin \alpha\pi}. \tag{4.14}$$

Proof. $f(z) := \frac{1}{(z-\alpha)^2 - \omega^2}$ is meromorphic on $\mathbb{C}$, has a finite number of poles and $\lim_{z\to\infty} zf(z) = 0$. Hence one can use the method of Prob. 4.6.1. J. Krzyż, "Zbiór zadań z funkcji analitycznych" involving integrating $\cot(\pi z)f(z)$ on a big square:

$$0 = \sum_{n=-\infty}^{\infty} \frac{2\mathrm{i}}{(n-\alpha)^2 - \omega^2} \tag{4.15}$$

$$+ 2\pi\mathrm{i}\mathrm{Res}\frac{\cot(\pi z)}{(z-\alpha)^2 - \omega^2}\Big|_{z=\alpha+\omega} + +2\pi\mathrm{i}\mathrm{Res}\frac{\cot(\pi z)}{(z-\alpha)^2 - \omega^2}\Big|_{z=\alpha-\omega} \tag{4.16}$$

$$= \sum_{n=-\infty}^{\infty} \frac{2\mathrm{i}}{(n-\alpha)^2 - \omega^2} + 2\pi\mathrm{i}\frac{\cot\pi(\omega+\alpha)}{2\omega} - 2\pi\mathrm{i}\frac{\cot\pi(\omega-\alpha)}{2\omega} \tag{4.17}$$

□

Proposition 4.2 *For $x \in [0, 2\pi]$,*

$$\sum_{n=-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(n-\alpha)x}}{(n-\alpha)^2 - \omega^2} = \frac{\pi\big(\sin(2\omega\pi - \omega x) + \mathrm{e}^{-2\mathrm{i}\alpha\pi}\sin(\omega x)\big)}{2\omega\sin((\alpha-\omega)\pi)\sin((\alpha+\omega)\pi)}. \tag{4.18}$$

Proof. Set

$$f(x) = f_{\omega,\alpha}(x) := \sum_{n=-\infty}^{\infty} \frac{\mathrm{e}^{\mathrm{i}(n-\alpha)x}}{(n-\alpha)^2 - \omega^2}.$$

We have

$$(\partial_x^2 + \omega^2)f(x) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(n-\alpha)x} = 2\pi\mathrm{e}^{-\mathrm{i}\alpha x} \sum_{m=-\infty}^{\infty} \delta(x - 2\pi m)), \tag{4.19}$$

In particular, (4.19) is zero in $]0, 2\pi[$. Hence $f(x) = a_+\mathrm{e}^{\mathrm{i}\omega x} + a_+\mathrm{e}^{-\mathrm{i}\omega x}$ there. Now

$$\begin{aligned} f(0) &= a_+ + a_- &&, \\ f(2\pi) &= a_+\mathrm{e}^{\mathrm{i}\omega 2\pi} + a_-\mathrm{e}^{-\mathrm{i}\omega 2\pi} = \mathrm{e}^{-\mathrm{i}\alpha 2\pi} f(0). \end{aligned}$$

Hence

$$\begin{aligned} a_- &= \frac{\mathrm{e}^{2\mathrm{i}\omega\pi} - \mathrm{e}^{-2\mathrm{i}\alpha\pi}}{\mathrm{e}^{2\mathrm{i}\omega\pi} - \mathrm{e}^{-2\mathrm{i}\omega\pi}} f(0), && (4.20) \\ a_+ &= \frac{-\mathrm{e}^{-2\mathrm{i}\omega\pi} + \mathrm{e}^{-2\mathrm{i}\alpha\pi}}{\mathrm{e}^{2\mathrm{i}\omega\pi} - \mathrm{e}^{-2\mathrm{i}\omega\pi}} f(0), && (4.21) \\ f(x) &= \frac{\big(\sin(2\omega\pi - \omega x) + \mathrm{e}^{-2\mathrm{i}\alpha\pi}\sin(\omega x)\big)}{\sin(2\omega\pi)} f(0) && (4.22) \\ &= \frac{\pi\big(\sin(2\omega\pi - \omega x) + \mathrm{e}^{-2\mathrm{i}\alpha\pi}\sin(\omega x)\big)}{2\omega\sin((\alpha-\omega)\pi)\sin((\alpha+\omega)\pi)}. && (4.23) \end{aligned}$$

□

4.8 Laplacian on an interval with twisted boundary conditions

Let H_κ be $-\partial_x^2$ on smooth functions on $[0, \pi]$ satisfying

$$\mathrm{e}^{\mathrm{i}\pi\kappa} f(0) = f(\pi), \quad \mathrm{e}^{\mathrm{i}\pi\kappa} f'(0) = f'(\pi). \tag{4.24}$$

Then H_κ defines a self-adjoint operator. From its eigenvectors one can form an o.n. basis

$$e_n(x) = \frac{1}{\sqrt{\pi}}\mathrm{e}^{\mathrm{i}(2n+\kappa)x}, \quad H_\kappa e_n = (2n+\kappa)^2 e_n, \quad n \in \mathbb{Z}. \tag{4.25}$$

Hence

$$\mathrm{sp} H_\kappa = \mathrm{sp}_{\mathrm{p}} H_\kappa = \{(2n+\kappa)^2 \; : \; n = 0, 1, 2, \dots\}.$$

The collowing cases are especially important:

(1) periodic $\kappa = 0$;

(2) antiperiodic, for $\kappa = 1$.

Set

$$R_\kappa(\omega^2, x, y) = (\omega^2 - H_\kappa)^{-1}(x, y)$$

Equation

$$(\partial_x^2 + \omega^2) R_\kappa(\omega^2, x, y) = \delta(x - y)$$

is solved by

$$R_\kappa(\omega^2, x, y) = \begin{cases} a_- \mathrm{e}^{\mathrm{i}x\omega} + b_- \mathrm{e}^{-\mathrm{i}x\omega}, & x < y; \\ a_+ \mathrm{e}^{\mathrm{i}x\omega} + b_+ \mathrm{e}^{-\mathrm{i}x\omega}, & x > y. \end{cases} \tag{4.26}$$

Let $y^\pm = y$, where we use the left- resp. right-sided limit. We get

$$R_\kappa(\omega^2, y^+, y) - R_\kappa(\omega^2, y^-, y) = 0, \tag{4.27}$$

$$\partial_x R_\kappa(\omega^2, y^+, y) - \partial_x R_\kappa(\omega^2, y^-, y) = 1, \tag{4.28}$$

$$\mathrm{e}^{\mathrm{i}\kappa\pi} R_\kappa(\omega^2, 0, y) = R_\kappa(\omega^2, \pi, y), \tag{4.29}$$

$$\mathrm{e}^{\mathrm{i}\kappa\pi} \partial_x R_\kappa(\omega^2, 0, y) = \partial_x R_\kappa(\omega^2, \pi, y). \tag{4.30}$$

We have 4 equations with 4 unknowns. According to W. Ciszewski this is solved by

$$R_\kappa(\omega^2, x, y) = \frac{\mathrm{i}}{2\omega} \begin{cases} \frac{\mathrm{e}^{\mathrm{i}\omega(y-x)}}{\mathrm{e}^{\mathrm{i}\pi(\omega+\kappa)}-1} - \frac{\mathrm{e}^{-\mathrm{i}\omega(y-x)}}{\mathrm{e}^{\mathrm{i}\pi(-\omega+\kappa)}-1}, & x < y; \\ \frac{\mathrm{e}^{\mathrm{i}\omega(x-y)}}{\mathrm{e}^{\mathrm{i}\pi(\omega-\kappa)}-1} - \frac{\mathrm{e}^{-\mathrm{i}\omega(y-x)}}{\mathrm{e}^{\mathrm{i}\pi(-\omega-\kappa)}-1}, & x > y. \end{cases} \tag{4.31}$$

Problem. Check (4.31) using (4.18) and

$$R_\kappa(\omega^2, x, y) = \sum_{n \in \mathbb{Z}} \frac{\mathrm{e}^{\mathrm{i}(2n+\kappa)(x-y)}}{\pi(\omega^2 - (2n+\kappa)^2)}. \tag{4.32}$$

4.9 Laplacian on an interval with Dirichlet and Neumann boundary conditions

Problem. Using (4.18) and (4.33),

$$R_{\mathrm{D}}(\omega^2)(x, y) = \sum_{n=1}^{\infty} \frac{2 \sin(xn) \sin(yn)}{\pi(\omega^2 - n^2)}, \tag{4.33}$$

check the following formula for the integral kernel of the resolvent of the Dirichlet Laplacian:

$$\begin{aligned} R_{\mathrm{D}}(\omega^2)(x, y) \quad = \quad & \frac{\sin \omega x \sin \omega(y - \pi) \theta(y - x)}{\omega \sin \omega\pi} \\ & + \frac{\sin \omega(x - \pi) \sin \omega y \theta(x - y)}{\omega \sin \omega\pi} \end{aligned}$$

Problem. Using (4.18) and (4.34)

$$R_{\mathrm{N}}(\omega^2)(x, y) = \frac{1}{\pi\omega^2} + \sum_{n=1}^{\infty} \frac{2 \cos(xn) \cos(yn)}{\pi(\omega^2 - n^2)}, \tag{4.34}$$

check the following formula for the integral kernel of the resolvent of the Neumann Laplacian:

$$R_{\mathrm{N}}(\omega^2)(x,y) = \frac{\cos\omega x\cos\omega(y-\pi)\theta(y-x)}{\omega\sin\omega\pi} + \frac{\cos\omega(x-\pi)\cos\omega y\theta(x-y)}{\omega\sin\omega\pi}.$$

4.10 Second order differential operators in one variable

Second order differential operators in one variable

$$\mathcal{C} := \sigma(x)\partial_x^2 + \tau(x)\partial_x \tag{4.35}$$

are especially important in applications. Often it is convenient to write them in a different form. Let $\rho(x)$ satisfy

$$\sigma(x)\rho'(x) = (\tau(x) - \sigma'(x))\rho(x). \tag{4.36}$$

Then

$$\mathcal{C} = \rho(x)^{-1}\partial_x\rho(x)\sigma(x)\partial_x. \tag{4.37}$$

Starting from now we assume that $-\infty \le a < b \le +\infty$, σ, ρ are real differentiable functions on $]a,b[$ and $\rho > 0$.

Theorem 4.3 *Let*

$$\mathcal{D} = \{f \in C^\infty(]a,b[) \ : \ f = 0 \ \ \textit{in a neighborhood of} \ \ a, b\}.$$

We define $\mathcal{C}$ as the operator on $\mathcal{D}$ given by (4.35). Then $\mathcal{C}$ is Hermitian in the sense of the Hilbert space $L^2(]a,b[,\rho)$.

Unfortunately, the above domain is usually too small to obtain an operator with eigenvalues.

4.11 Boundary conditions for the Sturm-Liouville problem

Let us consiser an operator given by the same differential formula, but on a greater domain. Under appropriate conditions it is still Hermitian:

Theorem 4.4 *Let $-\infty < a < b < +\infty$ and*

$$\sigma(a)\rho(a) = \sigma(b)\rho(b) = 0.$$

Then $\mathcal{C}$ is Hermitian on the domain $C^2([a,b])$ in the sense of the space $L^2(]a,b[,\rho)$

Proof.

$$\begin{aligned}
(g|\mathcal{C}f) &= \int_a^b \rho(x)\overline{g}(x)\rho(x)^{-1}\partial_x\sigma(x)\rho(x)\partial_x f(x)\mathrm{d}x \\
&= \int_a^b \overline{g}(x)\partial_x\sigma(x)\rho(x)\partial_x f(x)\mathrm{d}x \\
&= \overline{g(x)}\rho(x)\sigma(x)f'(x)\Big|_a^b - \int_a^b (\partial_x\overline{g}(x))\sigma(x)\rho(x)\partial_x f(x)\mathrm{d}x \\
&= -\overline{g'(x)}\rho(x)\sigma(x)f(x)\Big|_a^b + \int_a^b (\partial_x\rho(x)\sigma(x)\partial_x\overline{g(x)})f(x)\mathrm{d}x \\
&= \int_a^b \rho(x)\overline{(\rho(x)^{-1}\partial_x\sigma(x)\rho(x)\partial_x g(x))}f(x)\mathrm{d}x = (\mathcal{C}g|f).
\end{aligned}$$

□

Analogously we prove the following fact:

Theorem 4.5 *Let*

$$\lim_{x\to-\infty}\sigma(x)\rho(x)|x|^n = \lim_{x\to+\infty}\sigma(x)\rho(x)|x|^n = 0, \qquad n\in\mathbb{N}.$$

Then $\mathcal{C}$ is Hermitian on the domain consisting of polynomial functions in the sense of the space Hilbert $L^2(]-\infty,\infty[,\rho)$.

Obviously, similar statements hold for $]-\infty,b[$ and $]a,\infty[$.
Looking for eigenvalues of the operator $\mathcal{C}$ is often called the *Sturm-Liouville problem.*

5 Classical orthogonal polynomials

The following polynomials appear most often in applications:

Space	Polynomial	Equation
	Hermite polynomials	
$L^2(]-\infty,\infty[,\mathrm{e}^{-x^2})$	$H_n(x)=\frac{(-1)^n}{n!}\mathrm{e}^{x^2}\partial_x^n\mathrm{e}^{-x^2}$	$\partial_x^2-2x\partial_x+2n$
	Laguerre polynomials	
$L^2(]0,\infty[,x^\alpha\mathrm{e}^{-x})$ $\alpha>-1$	$L_n^\alpha(x)=\frac{1}{n!}\mathrm{e}^x x^{-\alpha}\partial_x^n\mathrm{e}^{-x}x^{n+\alpha}$	$x\partial_x^2+(\alpha+1-x)\partial_x+n$
	Jacobi polynomials	
$L^2(]-1,1[,(1-x)^\alpha(1+x)^\beta)$ $\alpha,\beta>-1$	$P_n^{\alpha,\beta}(x)=\frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}$ $\times\partial_x^n(1-x)^{\alpha+n}(1+x)^{\beta+n}$	$(1-x^2)\partial_x^2+(\beta-\alpha-(\alpha+\beta+2)x)\partial_x$ $+n(n+\alpha+\beta+1)$

We will try to explain why these polynomials are distinguished and are often called *classical orthogonal polynomials* (or even *very classical orthogonal polynomials*).

5.1 Hypergeometric class polynomials

We are looking for second order differential operators whose eigenfunctions are polynomials of all degrees.

Theorem 5.1 *Let*
$$\mathcal{C} := \sigma(z)\partial_z^2 + \tau(z)\partial_z + \eta(z) \tag{5.1}$$
be a differential operator such that there exist polynomials P_0, P_1, P_2 *of degree resp.* $0, 1, 2$ *satisfying*
$$\mathcal{C}P_n = \lambda_n P_n.$$
Then

(1) $\sigma(z)$ *is a polynomial of degree* ≤ 2,

(2) $\tau(z)$ *is a polynomial of degree* ≤ 1,

(3) $\eta(z)$ *is a polynomial of degree* ≤ 0 *(is a number).*

Proof. $\mathcal{C}P_0 = \eta(z)P_0$, hence $\deg\eta = 0$.
$\mathcal{C}P_1 = \tau(z)P_1' + \eta P_1$, so $\deg\tau \leq 1$.
$\mathcal{C}P_2 = \sigma(z)P_2'' + \tau(z)P_2'(z) + \eta P_2$, therefore, $\deg\sigma \leq 2$. □

It is thus enough to restrict our attention to operators of the form
$$\mathcal{C} := \sigma(z)\partial_z^2 + \tau(z)\partial_z, \tag{5.2}$$
where
$$\deg\sigma \leq 2, \qquad \deg\tau \leq 1. \tag{5.3}$$
We will show later that for a large class of (5.2) for all natural n there exists a polynomial of degree n which is an eigenfunction of (5.2).

Proposition 5.2 *Suppose that* σ *and* τ *are as above. Let polynomial* $P-K$ *of degree* k *satisfies*
$$\big(\sigma(z)\partial_z^2 + \tau(z)\partial_z + \lambda_k\big)P_k = 0. \tag{5.4}$$
Then
$$\frac{k(k-1)}{2}\sigma'' + k\tau' + \lambda_k = 0. \tag{5.5}$$

Proof. The kth derivative of (5.4) is (5.5) times $\partial_z^k P_k \neq 0$. □

5.2 Generalized Rodrigues formula

Many properties of polynomials eigenfunctions of operators described in Thm 5.1 can be derived in a unified way without separating the arguments into distinct cases. (This subsection can be skipped, all the material will be presented below for special cases).

Consider σ, τ satisfying (5.3). We fix σ, however we manifestly indicate the dependence on τ. Let ρ satisfy the equation

$$\sigma(z)\partial_z\rho(z) = \big(\tau(z) - \sigma'(z)\big)\,\rho(z). \tag{5.6}$$

Note that ρ can be expressed in terms of elementary functions. The operator $\mathcal{C}$ can be written as

$$\begin{aligned}\mathcal{C}(\tau) &= \rho^{-1}(z)\partial_z\sigma(z)\rho(z)\partial_z \\ &= \partial_z\rho^{-1}(z)\sigma(z)\partial_z\rho(z) - \tau' + \sigma''.\end{aligned} \tag{5.7}$$

Define

$$\begin{aligned}P_n(\tau; z) &:= \frac{1}{n!}\rho^{-1}(z)\partial_z^n\sigma^n(z)\rho(z) && (5.8)\\ &= \frac{1}{2\pi\mathrm{i}}\rho^{-1}(z)\int_{[0^+]}\sigma^n(z+t)\rho(z+t)t^{-n-1}\mathrm{d}t. && (5.9)\end{aligned}$$

Theorem 5.3 *We have* $\deg P_n(\tau) \leq n$,

$$\begin{aligned}\big(\sigma(z)\partial_z^2 + \tau(z)\partial_z\big)\,P_n(\tau; z) &= (n\tau' + n(n-1)\frac{\sigma''}{2})P_n(\tau; z), && (5.10)\\ \big(\sigma(z)\partial_z + \tau(z) - \sigma'(z)\big)\,P_n(\tau; z) &= (n+1)P_{n+1}(\tau - \sigma'; z), && (5.11)\\ \partial_z P_n(\tau; z) &= \left(\tau' + (n-1)\frac{\sigma''}{2}\right)P_{n-1}(\tau + \sigma'; z), && (5.12)\\ \frac{\rho(z + t\sigma(z))}{\rho(z)} &= \sum_{n=0}^{\infty} t^n P_n(\tau - n\sigma'; z). && (5.13)\end{aligned}$$

Proof. Introduce the following "creation and annihilation operators":

$$\begin{aligned}\mathcal{A}^+(\tau) : &= \sigma(z)\partial_z + \tau(z) = \rho^{-1}(z)\partial_z\rho(z)\sigma(z), \\ \mathcal{A}^- &:= \partial_z.\end{aligned}$$

Note that

$$\mathcal{A}^-\mathcal{A}^+(\tau - \sigma') - \mathcal{A}^+(\tau)\mathcal{A}^- = \tau' - \sigma'', \tag{5.14}$$

or more generally

$$\mathcal{A}^-\mathcal{A}^+\big(\tau + (k-1)\sigma'\big) - \mathcal{A}^+\big(\tau + k\sigma'\big)\mathcal{A}^- = \tau' - (k-1)\sigma''. \tag{5.15}$$

Using

$$\begin{array}{rcl}\mathcal{A}^+(\tau) & = & \rho^{-1}(z)\partial_z\rho(z)\sigma(z),\\ \mathcal{A}^+(\tau+\sigma') & = & \rho^{-1}(z)\sigma^{-1}(z)\partial_z\rho(z)\sigma^2(z),\\ \cdots & = & \cdots\\ \mathcal{A}^+(\tau+(n-1)\sigma') & = & \rho^{-1}(z)\sigma^{-(n-1)}\partial_z\rho(z)\sigma^n(z),\end{array}$$

we obtain

$$\mathcal{A}^+(\tau)\cdots\mathcal{A}^+(\tau+(n-1)\sigma')F_0 \quad = \quad \rho(z)^{-1}\partial_z^n\rho(z)\sigma^n(z)F_0(z).$$

Consider now $F_0 = 1$. We obtain

$$P_n(\tau, z) = \frac{1}{n!}\mathcal{A}^+(\tau)\cdots\mathcal{A}^+(\tau+(n-1)\sigma')1.$$

Now

$$\mathcal{A}^+(\tau-\sigma')P_n(\tau, z) = (n+1)P_{n+1}(\tau-\sigma', z)$$

is obvious, which yields (5.11). Using the commutation relations (5.15) we obtain

$$\begin{aligned}\mathcal{A}^-P_n(\tau, z) &= \frac{\big(\tau'+\tau'+\sigma''+\cdots+\tau'+(n-1)\sigma''\big)}{n!}\mathcal{A}^+\big(\tau+\sigma'\big)\cdots\mathcal{A}^+\big(\tau+(n-1)\sigma'\big)1\\ &= \frac{\big(n\tau'+\frac{n(n-1)}{2}\sigma''\big)}{n!}\mathcal{A}^+\big(\tau+\sigma'\big)\cdots\mathcal{A}^+\big(\tau+(n-1)\sigma'\big)1\\ &= \Big(\tau'+(n-1)\frac{\sigma''}{2}\Big)P_{n-1}(\tau+\sigma'),\end{aligned}$$

which yields (5.12). (5.11) i (5.12) imply (5.10). By the Taylor formula,

$$\rho(z+t\sigma(z)) = \sum_{n=0}^{\infty}\frac{t^n\sigma(z)^n}{n!}\partial_z^n\rho(z) = \rho(z)\sum_{n=0}^{\infty}t^nP_n(\tau-n\sigma'; z),$$

or (5.13). □

5.3 Classical orthogonal polynomials as eigenfunctions of Sturm-Liouville operators

We look for intervals $]a, b[\subset \mathbb{R}$ andd weights $]a, b[\ni x \mapsto \rho(x)$, for which there exist polynomials $P_0, P_1, \dots$ w satisfying $\deg P_n = n$,

$$\int \overline{P}_n(x)P_m(x)\rho(x)\mathrm{d}x = c_n\delta_{n,m} \tag{5.16}$$

and being eigenfunctions of a differential operator of second order $\mathcal{C} := \sigma(x)\partial_x^2 + \tau(x)\partial_x$, that is, for some $\lambda_n \in \mathbb{R}$

$$\left(\sigma(x)\partial_x^2 + \tau(x)\partial_x + \lambda_n\right)P_n(x) = 0. \tag{5.17}$$

(We allow $a = -\infty$ or $b = \infty$). To this end we want that the operator $\mathcal{C}$ is Hermitian in the sense of $L^2(]a, b[, \rho)$ on a domain containing polynomials. More precisely, we need to stisfy the following conditions:

(1) σ has to be a polynomial of degree at most 2 and τ a polynomial of degree at most 1. (See Thm 5.1).

(2) The weight ρ is a solution of the equation

$$\sigma(x)\rho'(x) = (\tau(x) - \sigma'(x))\rho(x), \tag{5.18}$$

is positive and σ real. This guarantees that $\mathcal{C}$, which can be written as

$$\mathcal{C} = \rho(x)^{-1}\partial_x \rho(x)\sigma(x)\partial_x,$$

is Hermitian in the sense of $L^2(]a,b[,\rho)$, at least on functions vanishing in neighborhoods of the endpoints of $]a,b[$. (See Thm 4.3).

(3) We want that $\mathcal{C}$ is Hermitian on a domain containing polynomials.

  (i) If an endpoint, say, a, is a finite number, then it is equivalent to the condition $\rho(a)\sigma(a) = 0$. (See Thm 4.4).

  (ii) If an endpoint is infinite, e.g. $a = -\infty$, then

$$\lim_{x\to-\infty} |x|^n \sigma(x)\rho(x) = 0$$

  should hold for any n.

In addition, P_n should belong to the Hilbert space $L^2(]a,b[,\rho)$ for any n, hence we demand that

$$\int_a^b \rho(x)|x|^n \mathrm{d}x < \infty. \tag{5.19}$$

The slightly stronger condition

$$\int_a^b \mathrm{e}^{\epsilon|x|}\rho(x)\mathrm{d}x < \infty \tag{5.20}$$

for some $\epsilon > 0$ is sufficient to obtain an orthonormal basis. (See Thm 2.1).

We will find all such weighted Hilbert spaces $L^2([a,b],\rho)$ for which such orthogonal polynomials exist. We will simplify our answer to standard forms

(1) by using the change of variables $x \mapsto ax + b$ for $a \neq 0$;

(2) by dividing (both the weight and the differential equation) by a constant

In this way we will obtain all classical orthogonal polynomials.

5.4 Classical orthogonal polynomials for $\deg\sigma = 0$

We can assume $\sigma(x) = 1$.

If $\deg\tau = 0$, then

$$\mathcal{C} = \partial_y^2 + c\partial_y.$$

It is easy to discard this case.

Hence $\deg\tau = 1$ and

$$\mathcal{C} = \partial_y^2 + (ay + b)\partial_y.$$

Let us substitute $x = \sqrt{\frac{|a|}{2}}\left(y + \frac{b}{a}\right)$. We obtain

$$\mathcal{C} = \partial_x^2 + 2x\partial_x, \qquad a > 0; \tag{5.21}$$

$$\mathcal{C} = \partial_x^2 - 2x\partial_x, \qquad a < 0. \tag{5.22}$$

This yields $\rho(x) = \mathrm{e}^{\pm x^2}$.

$\sigma(x)\rho(x) = \mathrm{e}^{\pm x^2}$ is never zero, hence the only possible interval is $]-\infty, \infty[$.

If $a > 0$, then $\rho(x) = \mathrm{e}^{x^2}$, which is impossible by (3ii).

If $a < 0$, then $\rho(x) = \mathrm{e}^{-x^2}$ and we obtain the Hermite operator. The interval $]-\infty, \infty[$ is admissible, and even satisfies (5.20). We obtain the equation and weight for Hermite polynomials, which will be discussed in the next subsection.

5.5 Hermite polynomials

Theorem 5.4 *Define*

$$H_n(x) = \frac{(-1)^n}{n!}\mathrm{e}^{x^2}\partial_x^n \mathrm{e}^{-x^2}.$$

Then H_n is a polynomial of degree n and is (up to a multiplicative constant) the only eigenfunction of the operator $\partial_x^2 - 2x\partial_x$ which is a polynomial of degree n. It satisfies the Hermite equation

$$(\partial_x^2 - 2x\partial_x + 2n)H_n(x) = 0.$$

and relations

$$(-\partial_x + 2x)H_n(x) = (n+1)H_{n+1}(x) \tag{5.23}$$

$$\partial_x H_n(x) = 2H_{n-1}(x), \tag{5.24}$$

$$\sum_{n=0}^{\infty} t^n H_n(x) = \mathrm{e}^{2tx - t^2}. \tag{5.25}$$

Proof. It is a consequence of Thm 5.3 for

$$\sigma(x) = -1, \quad \rho = \mathrm{e}^{-x^2}.$$

Below we present an independent proof. Let us introduce the "creation and annihilation operators"

$$\begin{aligned} A^- &= \partial_x, \\ A^+ &= -\partial_x + 2x = -\mathrm{e}^{x^2}\partial_x \mathrm{e}^{-x^2}. \end{aligned}$$

They satisfy the relations

$$[A^-, A^+] = 2. \tag{5.26}$$

We have $H_n = \frac{(A^+)^n 1}{n!}$. (Here, 1 denotes the vector in $L^2(\mathbb{R}, \mathrm{e}^{-x^2})$ given by the function equal to 1. On the other hand, in (5.26) 2 denotes the operator of multiplication by the number 2.) This implies

$$A^+ H_n = (n+1)H_{n+1}, \tag{5.27}$$

$$A^- H_n = 2H_{n-1}. \tag{5.28}$$

To prove (5.28), we use (5.26).

(5.27) and (5.28) show that

$$A^+A^-H_n = 2nH_n, \tag{5.29}$$
$$-\partial_x^2 + 2x\partial_x = A^+A^-. \tag{5.30}$$

Multiplying the definition of the Hermite polynomials by $t^n \mathrm{e}^{-x^2}$ we obtain

$$t^n \mathrm{e}^{-x^2} H_n(x) = \frac{(-t)^n}{n!}\partial_x^n \mathrm{e}^{-x^2}.$$

The Taylor formula yields

$$\mathrm{e}^{-x^2}\sum_{n=0}^{\infty} t^n H_n(x) = \mathrm{e}^{-(x-t)^2},$$

which implies (5.25). □

Theorem 5.5 $\{H_n \mid n \in \mathbb{N}_0\}$ *is an orthogonal basis in* $L^2(\mathbb{R}, \mathrm{e}^{-x^2})$ *with the normalization*

$$\int_{-\infty}^{\infty} H_n(x)^2 \mathrm{e}^{-x^2}\mathrm{d}x = \frac{\sqrt{\pi}2^n}{n!}.$$

Proof. Suppose that $n \geq m$. Then

$$\begin{aligned}\int_{-\infty}^{\infty} H_n(x)H_m(x)\mathrm{e}^{-x^2}\mathrm{d}x &= \frac{(-1)^n}{n!}\int_{-\infty}^{\infty}\left(\partial_x^n \mathrm{e}^{-x^2}\right)H_m(x)\mathrm{d}x \\ &= \frac{1}{n!}\int_{-\infty}^{\infty}\mathrm{e}^{-x^2}\partial_x^n H_m(x)\mathrm{d}x. \end{aligned} \tag{5.31}$$

(5.31) is 0 for $n > m$.

Let $n = m$. (5.24) and $H_0 = 1$ imply $\partial_x^n H_n(x) = 2^n$. Hence (5.31) is

$$\frac{2^n}{n!}\int_{-\infty}^{\infty}\mathrm{e}^{-x^2}\mathrm{d}x = \frac{2^n}{n!}\sqrt{\pi}.$$

□

Remark 5.6 *The definition of Hermite polynomials that we gave is consistent with the generalized Rodrigues formula (5.8). In the literature one can also find other conventions for Hermite polynomials, e.g.* $H_n(x) := (-1)^n \mathrm{e}^{x^2}\partial_x^n \mathrm{e}^{-x^2}$.

5.6 Classical orthogonal polynomials for $\deg\sigma = 1$

It is enough to consider the case $\sigma(y) = y$.

If $\deg\tau = 0$, then

$$\mathcal{C} = y\partial_y^2 + c\partial_y$$

But such a $\mathcal{C}$ always lowers the degree of a polynomial. Hence if $\mathcal{C}P = \lambda P$ for a certain polynomial, then $\lambda = 0$ and $P(x) = x^{-c+1}$. Thus we do not obtain polynomials of all degrees as eigenfunctions.

Hence $\deg\tau = 1$. Therefore, for $b \neq 0$,

$$y\partial_y^2 + (a + by)\partial_y. \tag{5.32}$$

After rescaling we obtian an operator that appears in the Laguerre equation

$$\mathcal{C} = -x\partial_x^2 + (-\alpha - 1 + x)\partial_x.$$

We check that $\rho = x^\alpha \mathrm{e}^{-x}$. $\rho(x)\sigma(x) = -x^{\alpha+1}\mathrm{e}^{-x}$ is zero only for $x = 0$ and $\alpha > -1$. The interval $[-\infty, 0]$ is ruled out by the condition (3ii). This condition allows for the interval $]0, \infty[$ for $\alpha > -1$, which then satisfies the condition 5.20.

We obtain the equation and weight for Laguerre polynomials, which will be discussed in the next subsection.

5.7 Laguerre polynomials

Theorem 5.7 *For $n \in \mathbb{N}$ and $\alpha \in \mathbb{C}$, set*

$$\begin{aligned} L_n^\alpha(x) &= \frac{1}{n!}\mathrm{e}^x x^{-\alpha}\partial_x^n \mathrm{e}^{-x}x^{n+\alpha} \\ &= \frac{(1+\alpha)_n}{n!}F(-n; 1+\alpha; x). \end{aligned}$$

Then L_n^α is a polynomial of degree n. It is a unique (up to a coefficient) eigenfunction of the operator $x\partial_x^2 + (\alpha+1-x)\partial_x$ which is a polynomial of degree n. L_n^α satisfy the Laguerre equation, which is the confluent equation with modified parameters:

$$\left(x\partial_x^2 + (\alpha + 1 - x)\partial_x + n\right) L_n^\alpha(x) = 0.$$

The following relations are true:

$$(x\partial_x + \alpha - x)L_n^\alpha(x) = (n+1)L_{n+1}^{\alpha-1}(x), \tag{5.33}$$

$$\partial_x L_n^\alpha(x) = -L_{n-1}^{\alpha+1}(x). \tag{5.34}$$

Proof. We can use Thm 5.3 for

$$\sigma(x) = x, \quad \rho(x) = \mathrm{e}^{-x}x^\alpha.$$

Below we present an independent proof.

Introduce "creation and annihilation operators"

$$\begin{aligned} A^- &= -\partial_x, \\ A^+_\alpha &= x\partial_x + \alpha - x = x^{-\alpha+1}\mathrm{e}^x\partial_x x^\alpha \mathrm{e}^{-x}. \end{aligned}$$

They satisfy the relations

$$A^- A^+_\alpha - A^+_{\alpha+1}A^- \;=\; 1. \tag{5.35}$$

We have

$$L_n^\alpha = \frac{A^+_{\alpha+1}\cdots A^+_{\alpha+n}1}{n!}. \tag{5.36}$$

(1 in (5.36) denotes the vector equal 1.) This implies

$$A^+_\alpha L_n^\alpha \;=\; (n+1)L_{n+1}^{\alpha-1}, \tag{5.37}$$

$$A^- L_n^\alpha \;=\; L_{n-1}^{\alpha+1}. \tag{5.38}$$

(5.38) follows by (5.35).

Finally, (5.37), (5.38) show

$$A^+_{\alpha+1}A^- L_n^\alpha = nL_n^\alpha. \tag{5.39}$$

Ale

$$-x\partial_x^2 - (\alpha+1-x)\partial_x = A^+_{\alpha+1}A^-. \tag{5.40}$$

□

Theorem 5.8 *If $\alpha > -1$, then Laguerre polynomials form an orthonormal basis in $L^2([0,\infty[, \mathrm{e}^{-x}x^\alpha)$ with the normalization*

$$\int_0^\infty L_n^\alpha(x)^2 x^\alpha \mathrm{e}^{-x}\mathrm{d}x = \frac{\Gamma(1+\alpha+n)}{n!}.$$

Proof. Let $n \geq m$. Then

$$\begin{aligned} \int_0^\infty L_n^\alpha(x)L_m^\alpha(x)x^\alpha \mathrm{e}^{-x}\mathrm{d}x &= \frac{1}{n!}\int_0^\infty \left(\partial_x^n x^{n+\alpha}\mathrm{e}^{-x}\right)L_m^\alpha(x)\mathrm{d}x \\ &= \frac{(-1)^n}{n!}\int_0^\infty x^{n+\alpha}\mathrm{e}^{-x}\partial_x^n L_m^\alpha(x)\mathrm{d}x. \end{aligned} \tag{5.41}$$

(5.41) is 0 for $n > m$.

Let $n = m$. By (5.34) and $L_0^\alpha = 1$ we obtain $\partial_x^n L_n^\alpha(x) = (-1)^n$. Hence (5.41) is

$$\frac{1}{n!}\int_0^\infty x^{n+\alpha}\mathrm{e}^{-x}\mathrm{d}x = \frac{\Gamma(n+\alpha+1)}{n!}.$$

□

5.8 Classical orthogonal polynomials for $\deg\sigma = 2$, σ has a double root

We can assume that $\sigma(x) = x^2$.

If $\tau(0) = 0$, then

$$\mathcal{C} = x^2\partial_x^2 + cx\partial_x.$$

Its eigenfunctions are polynomials x^n, but the weight $\rho(x) = x^{c-2}$ is not appropriate.

Let us assume that $\tau(0) \neq 0$. After rescaling we can assume that

$$\tau(x) = 1 + (\gamma + 2)x.$$

This yields $\rho(x) = \mathrm{e}^{-\frac{1}{x}}x^\gamma$. The only poin where $\rho(x)\sigma(x) = \mathrm{e}^{-\frac{1}{x}}x^{\gamma+2}$ can be zero is $x = 0$. Hence the only possible intervals are $]-\infty, 0[$ and $[0, \infty]$. Both are ruled out by (3ii).

5.9 Classical orthogonal polynomials for $\deg\sigma = 2$, σ has two roots

In this subsection we assume that the roots are distinct. If one of them is not real, then the other has to be its complex conjugate. Then it is enough to assume that $\sigma(x) = 1 + x^2$. We can suppose that $\tau(x) = a + (b + 2)x$. Then $\rho(x) = \mathrm{e}^{a \arctan x}(1 + x^2)^b$. $\sigma(x)\rho(x)$ is nowhere zero, and therefore the only possible interval is $]-\infty, \infty[$. This case has to be discarded, because $\lim_{|x|\to\infty} \rho(x)|x|^n(1 + x^2) = \infty$ for sufficiently large n.

Hence we can assume that the roots are distinct and real. It is enough to consider $\sigma(x) = 1 - x^2$. Let

$$\tau(x) = \beta - \alpha - (\alpha + \beta + 2)x.$$

We obtain $\rho(x) = |1 - x|^\beta|1 + x|^\alpha$. Similarly as above, the condition (3ii) rules out the intervals $]-\infty, -1[$ and $]1, \infty[$. What remains is the interval $[-1, 1]$, which satisfies (3i) for $\alpha, \beta > -1$. It leads to Jacobi polyn omials discussed in the next subsection.

5.10 Jacobi polynomials

Theorem 5.9 *Let $n \in \{0, 1, \dots\}$ and $\alpha, \beta \in \mathbb{C}$. Set*

$$\begin{aligned} P_n^{\alpha,\beta}(x) &= \frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\partial_x^n(1-x)^{\alpha+n}(1+x)^{\beta+n} && (5.42)\\ &= \frac{(1+\alpha)_n}{n!}F(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}). && (5.43) \end{aligned}$$

Then $P_n^{\alpha,\beta}$ satisfy the Jacobi equation, which is a slightly modified hypergeometric equation:

$$\big((1-x^2)\partial_x^2 + (\beta - \alpha - (\alpha+\beta+2)x)\partial_x + n(n+\alpha+\beta+1)\big)\, P_n^{\alpha,\beta}(x) = 0,$$

and the relations

$$\begin{aligned} \partial_x P_n^{\alpha,\beta}(x) &= \frac{\alpha+\beta+n+1}{2}P_{n-1}^{\alpha+1,\beta+1}, && (5.44)\\ -\frac{(1-x^2)\partial_x + \beta - \alpha - (\alpha+\beta)x}{2}P_n^{\alpha,\beta}(x) &= (n+1)P_{n+1}^{\alpha-1,\beta-1}(x). && (5.45) \end{aligned}$$

$$\sum_{n=0}^{\infty} P_n^{\alpha-n,\beta-n}(x)2^n t^n = \big(1+t(1+x)\big)^{\alpha}\big(1-t(1-x)\big)^{\beta}. \tag{5.46}$$

$P_n^{\alpha,\beta}$ is a polynomial of degree at most n. More precisely:

1. *If $\alpha+\beta \not\in \{-2n,\dots,-n-1\}$, then $\mathrm{deg} P_n^{\alpha,\beta}=n$. It is then up to a coefficient the unique eigensolution of the operator $\mathcal{C} := (1-x^2)\partial_x^2+(\beta-\alpha-(\alpha+\beta+2)x)\partial_x$, which is a polynomial of degree n.*
2. *If $\alpha+\beta \in \{-2n,\dots,-n-1\}$, but $\alpha \not\in \{-n,\dots,-1\}$ (or, equivalently, $\beta \not\in \{-n,\dots,-1\}$), then $\mathrm{deg} P_n^{\alpha,\beta} = -\alpha-\beta-n-1$.*
3. *If $\alpha+\beta \in \{-2n,\dots,-n-1\}$, but $\alpha \in \{-n,\dots,-1\}$ (or, equivalently, $\beta \in \{-n,\dots,-1\}$), then $P_n^{\alpha,\beta}=0$.*

Proof. We can use Thm 5.3 for

$$\sigma(x) = \frac{x^2-1}{2}, \quad \rho(x) = (1-x)^{\alpha}(1+x)^{\beta}.$$

Below we present an independent proof. Introduc the "creation and annihilation operators"

$$\begin{aligned}
A^- &= \partial_x, \\
A^+_{\alpha,\beta} &= -\frac{1}{2}\big((1-x^2)\partial_x+\beta-\alpha-(\alpha+\beta)x\big) \\
&= -\frac{1}{2}(1-x)^{-\alpha+1}(1+x)^{-\beta+1}\partial_x(1-x)^{\alpha}(1+x)^{\beta}.
\end{aligned}$$

They satisfy the relations

$$A^-A^+_{\alpha,\beta} - A^+_{\alpha+1,\beta+1}A^- = \frac{\alpha+\beta}{2}. \tag{5.47}$$

We have

$$P_n^{\alpha,\beta} = \frac{A^+_{\alpha+1,\beta+1}\cdots A^+_{\alpha+n,\beta+n}1}{n!}. \tag{5.48}$$

Hence,

$$A^+_{\alpha,\beta}P_n^{\alpha,\beta} = (n+1)P_{n+1}^{\alpha-1,\beta-1}, \tag{5.49}$$

$$A^-P_n^{\alpha,\beta} = \frac{\alpha+\beta+n+1}{2}P_{n-1}^{\alpha+1,\beta+1}. \tag{5.50}$$

To prove (5.50) we use (5.47) and sum up the arithmetic series.

Finally, (5.49), (5.50) shows

$$A^+_{\alpha+1,\beta+1}A^-P_n^{\alpha,\beta} = \frac{n(\alpha+\beta+n+1)}{2}P_n^{\alpha,\beta}. \tag{5.51}$$

Ale

$$-\frac{1}{2}(1-x^2)\partial_x^2+\frac{1}{2}(-\beta+\alpha+(\alpha+\beta)x)\partial_x = A^+_{\alpha+1,\beta+1}A^-. \tag{5.52}$$

Let us replace in the definition of Jacobi polynomials α, β with $\alpha - n, \beta - n$ and multiply them by $2^n t^n (1-x)^\alpha (1+x)^\beta$. We obtain

$$2^n t^n P_n^{\alpha-n,\beta-n}(x)(1-x)^\alpha(1+x)^\beta = \frac{(-t)^n}{n!}(1-x)^n(1+x)^n \partial_x^n (1-x)^\alpha (1+x)^\beta.$$

After summing up, the Taylor formula yields

$$(1-x)^\alpha(1+x)^\beta \sum_{n=0}^{\infty} 2^n t^n P_n^{\alpha-n,\beta-n}(x) = \big(1-x+t(1-x)(1+x)\big)^\alpha \big(1+x-t(1-x)(1+x)\big)^\beta,$$

which implies the formula for the generating function (5.46).

(5.44) and $P_0^{\alpha,\beta} = 1$ yield

$$\partial_x^n P_n^{\alpha,\beta}(x) = 2^{-n}(\alpha+\beta+n+1)\cdots(\alpha+\beta+2n). \tag{5.53}$$

Clearly, $\deg P_n^{\alpha,\beta} = n$ when the right hand side of (5.53) is different from zero.

Suppose that two polynomials P_1, P_2 of degree n satisfy

$$(\mathcal{C}+\eta_1)P_1 = (\mathcal{C}+\eta_2)P_2 = 0.$$

By Prop. 5.2,

$$\eta_1 = \eta_2 = n(n+\alpha+\beta+1).$$

Hence $P_1 - P_2$, a polynomial of degree $k \in \{0, 1, \dots, n-1\}$, solves the Jacobi equation. Applying again Prop. 5.2 we obtain

$$-k(k+\alpha+\beta+1) + n(n+\alpha+\beta+1) = 0.$$

This equation has two solutions: $k = n$ and $k = -n-\alpha-\beta-1 \notin \{0, 1, \dots, n-1\}$. The second soltion has to be discarded. $\square$

Theorem 5.10 *If $\alpha, \beta > -1$, then Jacobi polynomials form an orthogonal basis in $L^2([-1,1], (1-x)^\alpha(1+x)^\beta)$ with the normalization*

$$\int_{-1}^{1} (P_n^{\alpha,\beta}(x))^2 (1-x)^\alpha (1+x)^\beta \mathrm{d}x = \frac{\Gamma(1+\alpha+n)\Gamma(1+\beta+n)2^{\alpha+\beta+1}}{(1+2n+\alpha+\beta)n!\Gamma(1+\alpha+\beta+n)}. \tag{5.54}$$

Proof. Let $n \geq m$. Then

$$\begin{aligned} &\int_{-1}^{1} P_n^{\alpha,\beta}(x) P_m^{\alpha,\beta}(x)(1-x)^\alpha(1+x)^\beta \mathrm{d}x \\ = \quad & \frac{(-1)^n}{2^n n!} \int_{-1}^{1} \left(\partial_x^n (1-x)^{\alpha+n}(1+x)^{\beta+n}\right) P_m^{\alpha,\beta}(x)\mathrm{d}x \\ = \quad & \frac{1}{2^n n!} \int_{-1}^{1} (1-x)^{\alpha+n}(1+x)^{\beta+n} \partial_x^n P_m^{\alpha,\beta}(x)\mathrm{d}x. \end{aligned} \tag{5.55}$$

(5.55) is 0 for $n > m$.

Let $n = m$. Then (5.41) is

$$\begin{aligned}
&\frac{1}{2^{2n}n!}\int_{-1}^{1}(1-x)^{\alpha+n}(1+x)^{\beta+n}(\alpha+\beta+n+1)\cdots(\alpha+\beta+2n)\mathrm{d}x\\
=\ &\frac{2^{\alpha+\beta+1}}{n!}\int_{0}^{1}t^{\alpha+n}(1-t)^{\beta+n}(\alpha+\beta+n+1)\cdots(\alpha+\beta+2n)\mathrm{d}t\\
=\ &\frac{\Gamma(1+\alpha+n)\Gamma(1+\beta+n)2^{\alpha+\beta+1}}{(1+2n+\alpha+\beta)n!\Gamma(1+\alpha+\beta+n)}.
\end{aligned}$$

□

For each α, β we have a representation of $sl(2,\mathbb{C})$ on

$$P_0^{\alpha,\beta}, \dots, P_n^{\alpha-n,\beta-n}, \dots$$

(1) If $\alpha+\beta \notin \{0,1,2\dots\}$, this representation is irreducible and $\deg P_n^{\alpha-n,\beta-n} = n$.

(2) Let $\alpha+\beta \in \{0,1,2\dots\}$. Besides we suppose that $\alpha \notin \mathbb{Z}$ (equivalently, $\beta \notin \mathbb{Z}$),

$$\text{or}\quad \alpha \in \{\dots,-2,-1\}, \qquad \text{or}\quad \beta \in \{\dots,-2,-1\}.$$

Then this representation is reducible but indecomposable and we have

$$\deg P_n^{\alpha-n,\beta-n} = n, \qquad n = 0,1,\dots,\alpha+\beta; \tag{5.56}$$

$$\deg P_n^{\alpha-n,\beta-n} = n-(\alpha+\beta+1), \quad n \geq \alpha+\beta+1. \tag{5.57}$$

The space spanned by (5.57) is invariant. Besides, by (5.43),

$$P_{\alpha+\beta+1}^{-\beta-1,-\alpha-1} = \frac{(-\beta)_{\alpha+\beta+1}}{(\alpha+\beta+1)!} = \frac{(-\beta)(-\beta+1)\cdots(\alpha-1)\alpha}{(\alpha+\beta+1)!}. \tag{5.58}$$

(3) If $\alpha \in \{0,1,2\dots\}$ and $\beta \in \{0,1,\dots\}$, then

$$\deg P_n^{\alpha-n,\beta-n} = n, \qquad n = 0,1,\dots,\alpha+\beta; \tag{5.59}$$

$$P_n^{\alpha-n,\beta-n} = 0, \qquad n \geq \alpha+\beta+1. \tag{5.60}$$

and the space spanned by (5.59) is invariant. Besides,

$$P_n^{\alpha-n,\beta-n}(x) = \Big(\frac{x-1}{2}\Big)^{-\alpha+n}\Big(\frac{1+x}{2}\Big)^{-\beta+n}P_{\alpha+\beta-n}^{-\beta+n,\alpha+n}(x). \tag{5.61}$$

Proof of (5.61)**.** By (5.42),

$$P_n^{\alpha-n,\beta-n}(x) = \frac{2^n}{n!}\Big(\frac{x-1}{2}\Big)^{-\alpha+n}\Big(\frac{x+1}{2}\Big)^{-\beta+n}\partial_x^n\Big(\frac{x-1}{2}\Big)^{\alpha}\Big(\frac{x+1}{2}\Big)^{\beta}. \tag{5.62}$$

Setting $n=\alpha+\beta$ in (6.11) we obtain

$$P_{\alpha+\beta}^{-\beta,-\alpha}(x) = \frac{1}{2^{\alpha+\beta}(\alpha+\beta)!}(x-1)^{\beta}(1+x)^{\alpha}\partial_x^{\alpha+\beta}(x-1)^{\alpha}(1+x)^{\beta} \tag{5.63}$$

$$= \Big(\frac{x-1}{2}\Big)^{\beta}\Big(\frac{1+x}{2}\Big)^{\alpha} \tag{5.64}$$

By the recurrence relation (5.44) we obtain

$$P_{\alpha+\beta-n}^{-\beta+n,\alpha+n}(x) = \frac{2^n}{n!}\partial_x^n P_{\alpha+\beta}^{-\beta,-\alpha}(x) = \frac{2^n}{n!}\partial_x^n\Big(\frac{x-1}{2}\Big)^{\beta}\Big(\frac{x+1}{2}\Big)^{\alpha}. \tag{5.65}$$

Comparing (5.65) and (6.11) we obtain (5.61). □

Let us rewrite some of the identities, e.g. (5.54), in terms of the parameters $\alpha+\beta=2m$, $\alpha-\beta=2k$, $n=l-m$:

$$P_{l-m}^{k+m,-k+m}(w) = \frac{1}{(l-m)!}\Big(\frac{w-1}{2}\Big)^{-k-m}\Big(\frac{w+1}{2}\Big)^{k-m}\partial_w^{l-m}\Big(\frac{w-1}{2}\Big)^{l+k}\Big(\frac{w+1}{2}\Big)^{l-k}.$$

$$\big((1-w^2)\partial_w^2 - 2\big((m+1)w+k\big)\partial_w + (l-m)(l+m+1)\big)\, P_{l-m}^{k+m,-k+m}(w) = 0. \tag{5.66}$$

$$\partial_w P_{l-m}^{k+m,-k+m}(w) = \frac{1}{2}(l+m+1)P_{l-m-1}^{k+m+1,-k+m+1}(w), \tag{5.67}$$

$$\big((w^2-1)\partial_w + 2mw + 2k\big)P_{l-m}^{k+m,-k+m}(w) = 2(l-m+1)P_{l-m+1}^{k+m-1,-k+m-1}(w). \tag{5.68}$$

$$\int_{-1}^{1}(P_{l-m}^{m+k,m-k}(x))^2\Big(\frac{1-x}{2}\Big)^{m+k}\Big(\frac{1+x}{2}\Big)^{m-k}\mathrm{d}x = \frac{2\Gamma(1+l+k)\Gamma(1+l-k)}{(1+2l)(l-m)!\Gamma(1+l+m)}. \tag{5.69}$$

If $l=0,\frac{1}{2},1,\dots$ and $k,m=-l,\dots,l$,

$$P_{l-m}^{k+m,-k+m}(w) = \Big(\frac{w-1}{2}\Big)^{-m-k}\Big(\frac{w+1}{2}\Big)^{-m+k}P_{l+m}^{-k-m,k-m}(w) \tag{5.70}$$

$$= \frac{1}{(l+m)!}\partial_w^{l+m}\Big(\frac{w-1}{2}\Big)^{l-k}\Big(\frac{w+1}{2}\Big)^{l+k} \tag{5.71}$$

5.11 Ultraspherical polynomials (or Jacobi polynomials with $\alpha=\beta$)

Consider the special case of Jacobi polynomials for $\alpha=\beta=m$. To be consistent with later applications, we change the name of the variable from x to w. Thus,

$$\sigma(w) = \frac{w^2-1}{2}, \quad \rho(w) = (1-w^2)^m.$$

Theorem 5.11 *Set*

$$P_n^{m,m}(w) = \frac{(-1)^n}{2^n n!}(1-w^2)^{-m}\partial_w^n(1-w^2)^{m+n}$$

$$= \frac{(n+m)_n}{n!}F(-n, n+2m+1; m+1; \frac{1-w}{2}).$$

If
$$-2m \notin \{n+1,\dots,2n\}, \tag{5.72}$$
then $P_n^{m,m}$ are polynomials of degree n. They are then (up to a coefficient) the only eigensolution of the operator $\mathcal{C} := (1-w^2)\partial_w^2 - 2(m+1)w\partial_w$, which is a polynomial of degree n.

They satisfy the equation
$$\left((1-w^2)\partial_w^2 - 2(m+1)w)\partial_w + n(n+2m+1)\right) P_n^m(w) = 0.$$
and the relations
$$\begin{aligned} 2\partial_w P_n^{m,m}(w) &= (2m+n+1)P_{n-1}^{m+1,m+1}, &(5.73)\\ -\frac{(1-w^2)\partial_w - 2mw}{2} P_n^{m,m}(w) &= (n+1)P_{n+1}^{m-1,m-1}(w). &(5.74)\end{aligned}$$
$$\sum_{n=0}^{\infty} P_n^{m-n,m-n}(w)2^n t^n = \left(1+2tw+t^2(w^2-1)\right)^m. \tag{5.75}$$
$$P_n^{m,m}(1) = \frac{(m+1)_n}{n!}. \tag{5.76}$$

5.12 Legendre polynomials

Jacobi polynomials with $\alpha=\beta=0$ are especially important. We then have
$$\sigma(w) = \frac{w^2-1}{2}, \quad \rho(w) = 1.$$
They are called the Legendre polynomials:
$$P_l(w) := P_l^{0,0}(w) = \frac{(-1)^l}{2^l l!}\partial_w^l (1-w^2)^l.$$
They satisfy the Legendre equation
$$\left((1-w^2)\partial_w^2 - 2w\partial_w + l(l+1)\right) P_l(w) = 0. \tag{5.77}$$
They form an orthogonal basis of $L^2([-1,1])$ with the normalization
$$\int_{-1}^1 P_l(w)^2 \mathrm{d}w = \frac{2}{(1+2l)}.$$

We have $P_0 = 1$, $P_1(w) = w$, $P_2(w) = \frac{1}{2}(3w^2-1)$.

Theorem 5.12 *Legendre polynomials are the only polynomial solutions of the Legendre equation satisfying $P_l(1) = 1$.*

Proof. By induction we check that for $k=1,\dots,l$,
$$\partial_w^k (1-w^2)^l = (-1)^k (2w)^k l \cdots (l-k+1)(1-w^2)^{l-k} + C(w)(1-w^2)^{l-k+1},$$
where $C(w)$ is a polynomial. Setting $k=l$ and using the Rodrigues formula we obtain $P_l(1) = 1$.

Using the more general fact about the Jacobi equation we conclude that all polynomial solutions are proportional to P_l. □

6 Spherical harmonics on $\mathbb{S}^2$

6.1 Spherical coordinates in $\mathbb{R}^3$

Spherical coordinates in $\mathbb{R}^3$ are defined by

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta.$$

$$r = \sqrt{x^2+y^2+z^2}, \quad \theta = \arctan\frac{\sqrt{x^2+y^2}}{z}, \quad \phi = \arctan\frac{y}{x}.$$

The Jacobi matrix is

$$\begin{bmatrix} \frac{\partial r}{\partial x} & \frac{\partial r}{\partial y} & \frac{\partial r}{\partial z} \\ \frac{\partial \theta}{\partial x} & \frac{\partial \theta}{\partial y} & \frac{\partial \theta}{\partial z} \\ \frac{\partial \phi}{\partial x} & \frac{\partial \phi}{\partial y} & \frac{\partial \phi}{\partial z} \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \frac{\cos\theta\cos\phi}{r} & \frac{\cos\theta\sin\phi}{r} & -\frac{\sin\theta}{r} \\ -\frac{\sin\phi}{r\sin\theta} & \frac{\cos\phi}{r\sin\theta} & 0 \end{bmatrix}.$$

Instead of θ it is often convenient to use $w = \cos\theta = \frac{z}{\sqrt{x^2+y^2+z^2}}$. Note that

$$\partial_\theta = (1-w^2)^{\frac{1}{2}}\partial_w.$$

Spherical coordinates can be treated as a map

$$]0,\infty[\times\mathbb{S}^2 \to \mathbb{R}^3\backslash\{0\}$$

where $(w,\phi) \in]-1,1[\times[0,2\pi[$ parametrizes $\mathbb{S}^2$ without both poles. Its Jacobian is $r^2\mathrm{d}r\mathrm{d}w\mathrm{d}\phi = r^2\sin\theta\mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi$. The standard measure on the sphere is $\sin\theta\mathrm{d}\theta\mathrm{d}\phi = \mathrm{d}w\mathrm{d}\phi$.

The Laplacian in spherical coordinates is

$$\begin{aligned} \Delta =& \partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\Big(\frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta + \frac{\partial_\phi^2}{\sin^2\theta}\Big) \\ =& \partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^2}. \end{aligned} \tag{6.1}$$

$\Delta_{\mathbb{S}^2}$ is the operator acting on $\mathbb{S}^2$ called the *Laplace–Beltrami operator on the sphere.* It is

$$\begin{aligned} \Delta_{\mathbb{S}^2} &= \frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta + \frac{\partial_\phi^2}{\sin^2\theta} \\ &= \partial_w(1-w^2)\partial_w + \frac{\partial_\phi^2}{1-w^2} && (6.2) \\ &= (1-w^2)\partial_w^2 - 2w\partial_w + \frac{\partial_\phi^2}{1-w^2}, && (6.3) \end{aligned}$$

Proposition 6.1 $\Delta_{\mathbb{S}^2}$ *with domain $C^\infty(\mathbb{S}^2)$ is Hermitian in the sense of the Hilbert space $L^2(\mathbb{S}^2)$.*

Proof. We can identify $L^2(\mathbb{S}^2)$ with $L^2([-1,1]\times[0,2\pi[)$ with help of the coordinates w,ϕ. Using (6.2), integrating by parts and taking into account that we have periodic boundary conditions in ϕ we obtain

$$\begin{aligned}
-(f|\Delta_{\mathbb{S}^2}g) &= \int_{-1}^{1}\mathrm{d}w\int_0^{2\pi}\mathrm{d}\phi\Big(\overline{\partial_w f(w,\phi)}(1-w^2)\partial_w g(w,\phi)+\frac{1}{1-w^2}\overline{\partial_\phi f(w,\phi)}\partial_\phi g(w,\phi)\Big)\\
&= -(\Delta_{\mathbb{S}^2}f|g).
\end{aligned}$$

□

6.2 Reminder about ultraspherical polynomials

We will need Jacobi polynomials for $\alpha=\beta=m$. In view of their applications to spherical harmonics it is convenient to write their degree as $n=l-m$:

$$P_{l-m}^{m,m}(w) \;=\; \frac{(-1)^{l-m}}{2^{l-m}(l-m)!}(1-w^2)^{-m}\partial_w^{l-m}(1-w^2)^l.$$

They satisfy the equation

$$\big((1-w^2)\partial_w^2-2(m+1)w\partial_w+(l-m)(l+m+1)\big)\,P_{l-m}^{m,m}(w)=0. \tag{6.4}$$

Adapted to the present notation, the recurrence relations for $P_n^{m,m}$ read

$$\begin{aligned}
2\partial_w P_{l-m}^{m,m}(w) &= (l+m+1)P_{l-m-1}^{m+1,m+1}(w), &(6.5)\\
-\frac{1}{2}\big((1-w^2)\partial_w-2m\big)P_{l-m}^{m,m}(w) &= (l-m+1)P_{l-m+1}^{m-1,m-1}(w). &(6.6)
\end{aligned}$$

For $m>-1$ and $l=m,m+1,m+2,\dots$ they form an o.n. basis of $L^2([-1,1],(1-w^2)^m)$ with the normalization

$$\begin{aligned}
\int_{-1}^{1}P_{l-m}^{m,m}(w)^2(1-w^2)^m\mathrm{d}w &= \frac{\Gamma(1+l)^2 2^{2m+1}}{(1+2l)(l-m)!\Gamma(1+l+m)} &(6.7)\\
&= \frac{(l!)^2 2^{2m+1}}{(1+2l)(l-m)!(l+m)!}, &(6.8)
\end{aligned}$$

where in (6.8) we assume that l,m are integers.

Theorem 6.2 *Let $l=0,1,\dots,$ $m\in\mathbb{Z}$. Then Jacobi polynomials satisfy*

$$\begin{aligned}
(-1)^m\Big(\frac{1-w^2}{4}\Big)^{\frac{m}{2}}P_{l-m}^{m,m}(w) &= \frac{(-1)^l}{2^l(l-m)!}(1-w^2)^{-\frac{m}{2}}\partial_w^{l-m}(1-w^2)^l\\
=\;\Big(\frac{1-w^2}{4}\Big)^{-\frac{m}{2}}P_{l+m}^{-m,-m}(w) &= \frac{(-1)^{l+m}}{2^l(l+m)!}(1-w^2)^{\frac{m}{2}}\partial_w^{l+m}(1-w^2)^l \qquad (6.9)
\end{aligned}$$

If in addition $m<-l$ or $l<m$, then (6.9) is 0.

This is a special case of (5.61). Below we present an independent proof.

Lemma 6.3 *The term at the highest power of $P_{l-m}^{m,m}(w)$ is $w^{l-m}\frac{\Gamma(2l+1)}{2^{l-m}(l-m)!\Gamma(l+m+1)}$.*

Proof. For large w

$$\begin{aligned} P_{l-m}^{m,m}(w) &= \frac{(-1)^{l-m}}{2^{l-m}(l-m)!}(-w^2)^{-m}\partial_w^{l-m}(-w^2)^l \\ &= w^{l-m}\frac{2l\cdots(l+m+1)}{2^{l-m}(l-m)!}. \end{aligned}$$

Proof of Thm 6.2. Note first that

$$\begin{aligned} &(1-w^2)^m\left((1-w^2)\partial_w^2 - 2(m+1)w\partial_w + (l-m)(l+m+1)\right)(1-w^2)^{-m} \\ = &\left((1-w^2)\partial_w^2 - 2(-m+1)w\partial_w + (l+m)(l-m+1)\right). \end{aligned} \tag{6.10}$$

Hence the operator (6.10) anihilates both $(1-w^2)^m P_{l-m}^{m,m}(w)$ and $P_{l+m}^{-m,-m}(w)$.

Assume first that $m \geq 0$. Both functions are polynomials, the first has the highest term $w^{l-m+2m}(-1)^m\frac{(2l)!}{2^{l-m}(l-m)!(l+m)!}$, the secon has the highest term $w^{l+m}\frac{(2l)!}{2^{l+m}(l-m)!(l+m)!}$. The condition (5.72) is satisfied, hence by the uniqueness of polynomial solutions of the Jacobi equation both functions are proportional to one another.

Next we note that the identities (6.9) do not change if we replace m with $-m$. Hence the theorem is true also for $m \leq 0$.

If $m < -l$, then $P_{l+m}^{m,m} = 0$, and if $l < m$, then $P_{l-m}^{m,m} = 0$. $\square$

In applications, equation (6.4) is often transformed as follows

$$\begin{aligned} &(1-w^2)^{\frac{m}{2}}\left((1-w^2)\partial_w^2 - (2+2m)w\partial_w + (l-m)(l+m+1)\right)(1-w^2)^{-\frac{m}{2}} \\ = &(1-w^2)\partial_w^2 - 2w\partial_w - \frac{m^2}{1-w^2} + l(l+1). \end{aligned} \tag{6.11}$$

The equation given by (6.11) is called the *associated Legendre equation.*

6.3 Standard basis of spherical harmonics in $L^2(S^2)$

Spherical harmonics are defined as eigenfuctions of the Laplace-Beltrami operator. That is,

$$(\Delta_{\mathbb{S}^2} + \lambda)Y = 0. \tag{6.12}$$

We make the ansatz $Y(\theta,\phi) = f(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi}$. We obtain the equation

$$\left(\partial_w(1-w^2)\partial_w - \frac{m^2}{1-w^2} + \lambda\right)f(w) = 0, \tag{6.13}$$

which is recognized to be the associated Legendre equation with $\lambda = l(l+1)$. Setting $f(w) = (1-w^2)^{\frac{m}{2}}p(w)$ we obtain the Jacobi equation

$$\left((1-w^2)^{\frac{m}{2}}\left((1-w^2)\partial_w^2 - (2+2m)w\partial_w + (l-m)(l+m+1)\right)(1-w^2)^{-\frac{m}{2}}\right)p(w) = 0. \tag{6.14}$$

Hence

$$(-1)^m \mathrm{e}^{\mathrm{i}m\phi}(1-w^2)^{\frac{m}{2}} P_{l-m}^{m,m}(w) = \mathrm{e}^{\mathrm{i}m\phi}(1-w^2)^{-\frac{m}{2}} P_{l+m}^{-m,-m}(w). \tag{6.15}$$

are eigenfunctions of $\Delta_{\mathbb{S}^2}$ with eigenvalues $l(l+1)$, where

$$m = -l, -l+1, \dots, l. \tag{6.16}$$

They are called *spherical harmonics of degree l*.

One of standard normalizations of harmonics (6.15) is

$$\begin{aligned} Y_{l,m}(w,\phi) &= (-1)^m \frac{\sqrt{(l+m)!(l-m)!}}{l!} \Big(\frac{1-w^2}{4}\Big)^{\frac{m}{2}} P_{l-m}^{m,m}(w)\mathrm{e}^{\mathrm{i}m\phi} \\ &= \frac{\sqrt{(l+m)!(l-m)!}}{l!} \Big(\frac{1-w^2}{4}\Big)^{-\frac{m}{2}} P_{l+m}^{-m,-m}(w)\mathrm{e}^{\mathrm{i}m\phi}. \end{aligned} \tag{6.17}$$

Theorem 6.4 *The functions $Y_{l,m}$ for (6.16) form an o.n. basis of $L^2(\mathbb{S}^2)$ satisfying*

$$\int_0^\pi \sin\theta \mathrm{d}\theta \int_{-\pi}^{\pi} \mathrm{d}\phi \, |Y_{l,m}(\cos(\theta),\phi)|^2 = \frac{4\pi}{1+2l}.$$

Proof. Let

$$\begin{aligned} e_m &:= \mathrm{e}^{\mathrm{i}m\phi}, & (6.18) \\ f_{m,l} &:= \epsilon_m \sqrt{\frac{(l+1)\cdots(l+|m|)}{(l-|m|+1)\cdots l}} 2^{-|m|}(1-w^2)^{\frac{|m|}{2}} P_{l-|m|}^{|m|,|m|}(w), & (6.19) \end{aligned}$$

where $\epsilon_m = 1$ for $m \le 0$ and $\epsilon_m = (-1)^m$ for $m \ge 0$. We have then

$$Y_{l,m}(w,\phi) = f_{m,l} \otimes e_m. \tag{6.20}$$

Clearly, e_m, $m \in \mathbb{Z}$, form an o.n. basis of $L^2([-\pi,\pi], \mathrm{d}\phi)$.

Let us fix for a moment $m = 0, 1, \dots$. Then for $l, l' \ge m$,

$$\int_{-1}^{1} P_{l-m}^{m,m}(w) P_{l'-m}^{m,m}(w)(1-w^2)^m \mathrm{d}w = \delta_{l,l'} \frac{2^{2m+1} l \cdots (l-m+1)}{(1+2l)(l+1)\cdots(l+m)}.$$

(See (6.8)). Therefore, $f_{m,l}$, $l = m, m+1, \dots$, is an orthogonal basis of $L^2([0,\pi], \mathrm{d}w)$.

Hence

$$f_{m,l} \otimes e_m, \quad m \in \mathbb{Z}, \quad l = m, m+1, \dots$$

is an orthogonal basis of

$$L^2([0,\pi], \mathrm{d}w) \otimes L^2([-\pi,\pi], \mathrm{d}\phi) \simeq L^2([0,\pi] \times [-\pi,\pi], \mathrm{d}w\mathrm{d}\phi) \simeq L^2(\mathbb{S}^2).$$

□

The following special cases are important:

$$Y_{l,0}(\cos\theta,\phi) = P_l(\cos\theta), \tag{6.21}$$

$$Y_{l,\pm l}(\cos\theta,\phi) = (-1)^l \sqrt{\frac{(2l)!}{l!}} \frac{\sin^l\theta}{2^l} \mathrm{e}^{\pm \mathrm{i}l\phi}. \tag{6.22}$$

6.4 Lie group $SO(3)$

The group $SO(3)$ acts on $\mathbb{R}^3$ and on $\mathbb{S}^2$. It also acts on functions on $\mathbb{R}^3$ and on $\mathbb{S}^2$:

$$R_* f(x) = f(R^{-1}x). \tag{6.23}$$

In particular, we have the rotations

Introduce the generators of rotation L_x, L_y, L_y. We first describe them in the Cartesian coordinates, and then in the spherical coordinates:

$$\begin{aligned}
L_x &= y\partial_z - z\partial_y &&= -\sin\phi\partial_\theta - \frac{\cos\theta\cos\phi}{\sin\theta}\partial_\phi \\
& &&= -\sin\phi\sqrt{1-w^2}\partial_w + \frac{w}{\sqrt{1-w^2}}\cos\phi\partial_\phi, \\
L_y &= z\partial_x - x\partial_z &&= -\cos\phi\partial_\theta - \frac{\cos\theta\sin\phi}{\sin\theta}\partial_\phi \\
& &&= \cos\phi\sqrt{1-w^2}\partial_w + \frac{w}{\sqrt{1-w^2}}\sin\phi\partial_\phi, \\
L_z &= x\partial_y - y\partial_x &&= \partial_\phi.
\end{aligned}$$

Their exponentials are rotations in the x, y and z axis:

$$\left(\mathrm{e}^{\theta L_x} f\right)(x,y,z) = f(x, \cos\theta y + \sin\theta z, \sin\theta y - \cos\theta z), \tag{6.24}$$

$$\left(\mathrm{e}^{\theta L_y} f\right)(x,y,z) = f(\sin\theta z - \cos\theta x, y, \cos\theta z + \sin\theta x), \tag{6.25}$$

$$\left(\mathrm{e}^{\theta L_z} f\right)(x,y,z) = f(\cos\theta x + \sin\theta y, \sin\theta x - \cos\theta y, z). \tag{6.26}$$

The operators L_x, L_y, L_z span the Lie algebra $so(3)$:

$$[L_x, L_y] = -L_z, \quad [L_y, L_z] = -L_x, \quad [L_z, L_x] = -L_y. \tag{6.27}$$

We also have the generator of dilations:

$$A = x\partial_x + y\partial_y + z\partial_z = r\partial_r. \tag{6.28}$$

A commutes with L_x, L_y, L_z.

Direct calculations show that

$$\Delta_{\mathbb{S}^2} = L_x^2 + L_y^2 + L_z^2.$$

This can be also seen quite simply, almost without using spherical coordinates. First we easily check that $A = r\partial_r$. Then we compute

$$r^2\Delta = A(A+1) + L_x^2 + L_y^2 + L_z^2 \tag{6.29}$$

and compare this with (6.1).

The operator $\Delta_{\mathbb{S}^2}$ is invariant wrt the group $SO(3)$. Therefore, it commutes with $L_x, L_y, , L_z$. This can be also easily checked directly. Therefore, L_x, L_y and L_z preserve eigenspaces of $\Delta_{\mathbb{S}^2}$.

Spherical harmonics are chosen so that they diagonalize simultaneously $-\Delta_{\mathbb{S}^2}$ and L_z:

$$-\Delta_{\mathbb{S}^2} Y_{lm} = l(l+1)Y_{lm}, \quad -\mathrm{i}L_z Y_{lm} = mY_{lm}. \tag{6.30}$$

Clearly, the following operators preserve the eigenspaces of $\Delta_{\mathbb{S}^2}$:

$$L_+ \ := \mathrm{i}(L_x + \mathrm{i}L_y) \ = -(1-w^2)^{\frac{1}{2}}\partial_w \mathrm{e}^{\mathrm{i}\phi} + \mathrm{i}\frac{w}{(1-w^2)^{\frac{1}{2}}}\mathrm{e}^{\mathrm{i}\phi}\partial_\phi, \tag{6.31}$$

$$L_- \ := \mathrm{i}(L_x - \mathrm{i}L_y) \ = (1-w^2)^{\frac{1}{2}}\partial_w \mathrm{e}^{-\mathrm{i}\phi} + \mathrm{i}\frac{w}{(1-w^2)^{\frac{1}{2}}}\mathrm{e}^{-\mathrm{i}\phi}\partial_\phi. \tag{6.32}$$

(6.27) imply

$$[-\mathrm{i}L_z, L_\pm] = \pm L_\pm, \tag{6.33}$$

$$[L_+, L_-] = -2\mathrm{i}L_z. \tag{6.34}$$

Hence if $|m)$ is an eigenvector of $-\mathrm{i}L_z$ with eigenvalue m, then $L_\pm|m)$ is an eigenvector of $-\mathrm{i}L_z$ with eigenvalue $m \pm 1$.

Using

$$(1-w^2)^{\pm\frac{m+1}{2}}\partial_w(1-w^2)^{\mp\frac{m}{2}} = (1-w^2)^{\frac{1}{2}}\partial_w \pm m\frac{w}{(1-w^2)^{\frac{1}{2}}}, \tag{6.35}$$

we can rewrite (6.5) and (6.6) in the form

$$\begin{aligned}
\left((1-w^2)^{\frac{1}{2}}\partial_w + m\frac{w}{(1-w^2)^{\frac{1}{2}}}\right)\frac{(1-w^2)^{\frac{m}{2}}}{2^m}P_{l-m}^{m,m}(w) &= (l+m+1)\frac{(1-w^2)^{\frac{m+1}{2}}}{2^{m+1}}P_{l-m-1}^{m+1,m+1}(w),\\
\left(-(1-w^2)^{\frac{1}{2}}\partial_w + m\frac{w}{(1-w^2)^{\frac{1}{2}}}\right)\frac{(1-w^2)^{\frac{m}{2}}}{2^m}P_{l-m}^{m,m}(w) &= (l-m+1)\frac{(1-w^2)^{\frac{m-1}{2}}}{2^{m-1}}P_{l-m+1}^{m-1,m-1}(w).
\end{aligned}$$

Therefore

$$\begin{aligned}
-\mathrm{i}L_z Y_{l,m} &= mY_{l,m},\\
L_+ Y_{l,m} &= \sqrt{(l-m)(l+m+1)}Y_{l,m+1},\\
L_- Y_{l,m} &= \sqrt{(l+m)(l-m+1)}Y_{l,m-1}.
\end{aligned} \tag{6.36}$$

6.5 Spherical harmonics as a basis of a representation of $so(3)$

It is well known that irreducible representations of $so(3)$ can be labelled by the spin l, which can take values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$. Only for integer spins these representations can be integrated to representations of the group $SO(3)$. These representations can be realized in the space of polynomials of degree $2l$ with basis

$$\begin{aligned}
u_{l,m} &:= \frac{(2l)!}{(l-m)!(l+m)!}z_-^{l-m}z_+^{l+m}, \qquad m = -l, -l+1, \dots, l;\\
-\mathrm{i}L_z &:= \frac{1}{2}(z_+\partial_{z_+} - z_-\partial_{z_-}),\\
L_- &:= z_-\partial_{z_+},\\
L_+ &:= z_+\partial_{z_-}.
\end{aligned}$$

(Note that this definition gives automatically $u_{l,m} = 0$ for $m = -l-1, -l-2, \dots$ and $m = l+1, l+2, \dots$, because $\frac{1}{n!} = 0$ for $n = -1, -2, \dots$). We have

$$\begin{aligned}
-\mathrm{i}L_z u_{l,m} &= m u_{l,m}, \\
L_+ u_{l,m} &= (l+m+1) u_{l,m+1}, \\
L_- u_{l,m} &= (l-m+1) u_{l,m-1}.
\end{aligned} \tag{6.37}$$

We will show that properly normalized spherical harmonics realize this representation. Let us change the normalization of spherical harmonics:

$$\mathcal{Y}_{l,m}(w,\phi) := (-1)^m \frac{(1-w^2)^{\frac{m}{2}}}{2^m} P_{l-m}^{m,m}(w) \mathrm{e}^{\mathrm{i}m\phi} \tag{6.38}$$

$$= \frac{(1-w^2)^{-\frac{m}{2}}}{2^{-m}} P_{l+m}^{-m,-m}(w) \mathrm{e}^{\mathrm{i}m\phi}. \tag{6.39}$$

The standard spherical harmonics differ from $\mathcal{Y}_{l,m}$ by appropriate coefficients:

$$Y_{l,m}(w,\phi) = \frac{\sqrt{(l+m)!(l-m)!}}{l!} \mathcal{Y}_{l,m}(w,\phi). \tag{6.40}$$

We obtain relations identical with (6.37):

$$\begin{aligned}
-\mathrm{i}L_z \mathcal{Y}_{l,m} &= m \mathcal{Y}_{l,m}, \\
L_+ \mathcal{Y}_{l,m} &= (l+m+1) \mathcal{Y}_{l,m+1}, \\
L_- \mathcal{Y}_{l,m} &= (l-m+1) \mathcal{Y}_{l,m-1}.
\end{aligned} \tag{6.41}$$

6.6 Legendre functions

We introduced the standard basis of spherical harmonics with help of Jacobi polynomials. In literature usually one can usually find a different, less convenient definition based on the so-called associated Legendre functions, which are solutions of the associated Legendre equation (6.13). In the literature one can find two varieties of these functions:

$$\begin{aligned}
P_l^m(w) &:= \frac{2^m (l+m)!}{l!} (1-w^2)^{-\frac{m}{2}} P_{l+m}^{-m,-m}(w) \\
&= \frac{(-1)^{m+l}}{2^l l!} (1-w^2)^{\frac{m}{2}} \partial_w^{l+m} (1-w^2)^l, \\
\text{or} \qquad P_l^m(w) &:= (-1)^m \frac{2^m (l+m)!}{l!} (1-w^2)^{-\frac{m}{2}} P_{l+m}^{-m,-m}(w) \\
&= \frac{(-1)^l}{2^l l!} (1-w^2)^{\frac{m}{2}} \partial_w^{l+m} (1-w^2)^l,
\end{aligned}$$

The first variety uses the so-called Condon-Shockley convention, which we will adhere.

For $m \geq 0$ associated Legendre functions can be expressed in terms of Legendre polynomials:

$$P_l^m(w) := (-1)^m (1-w^2)^{\frac{m}{2}} \partial_w^m P_l(w),$$

We have the identity:

$$P_l^{-m}(w) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(w).$$

Here are spherical harmonics expressed in terms of associated Legendre functions:

$$Y_{l,m}(w,\phi) = \mathrm{e}^{\mathrm{i}m\phi} \sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(w).$$

6.7 Projection onto lth degree spherical harmonics

Consider the Hilbert space $L^2(\mathbb{S}^2)$. Let $\mathbb{P}_l$ denote the orthogonal projection onto spherical harmonics of degree l. In other words,

$$-\Delta_{\mathbb{S}^2} = \sum_{l=0}^{\infty} l(l+1)\mathbb{P}_l.$$

We can assume that they are given by an integral kernel

$$\mathbb{P}_l f(\xi) = \int \mathbb{P}_l(\xi,\eta) f(\eta) \mathrm{d}\eta,$$

wheree $\xi, \eta \in \mathbb{S}^2$ and $\mathrm{d}\eta$ denotes the standard measure on the sphere.

Proposition 6.5

$$\mathbb{P}_l(\xi,\eta) = \frac{2l+1}{4\pi} P_l(\xi \cdot \eta). \tag{6.42}$$

Proof. $\mathbb{P}_l(\xi,\eta)$ is invariant wrt rotations. Hence it depends only on the angle between ξ and η.
Note that

$$-\Delta_{\mathbb{S}^2}\mathbb{P}_l = l(l+1)\mathbb{P}_l.$$

On the level of the integral kernel it means

$$-\Delta_{\mathbb{S}^2}\mathbb{P}_l(\xi,\eta) = l(l+1)\mathbb{P}_l(\xi,\eta),$$

where the operator $\Delta_{\mathbb{S}^2}$ acts on the variable ξ. Hence,for a fixed η, the function $\xi \mapsto \mathbb{P}_l(\xi,\eta)$ is a spherical harmonics of degree l invariant wrt rotations around η.

If we set $\eta = (0,0,1)$, then $\mathbb{P}_l\big(\xi,(0,0,1)\big)$ is invariant wrt rotations in the z axis. In other words, it depends only on the z-component ofj ξ, that is on $w = \xi \cdot (1,0,0)$. Spherical harmonics of degree l invariant wrt rotations in the z axis are proportional to $Y_{l,0}$, which is proportional to the Legendre polynomial $P_l(w)$. Hence,

$$\mathbb{P}_l\big(\xi,(0,0,1)\big) = c_l P_l(w), \tag{6.43}$$

$$\text{or } \mathbb{P}_l(\xi,\eta) = c_l P_l(\xi \cdot \eta). \tag{6.44}$$

$\mathbb{P}_l$ is a projection, therefore

$$\mathbb{P}_l^2 = \mathbb{P}_l,$$

which yields

$$\int \mathbb{P}_l(\xi,\eta)\mathbb{P}_l(\eta,\zeta)\mathrm{d}\eta = \mathbb{P}_l(\xi,\zeta).$$

Setting $\xi = \zeta = (0,0,1)$ we obtain

$$c_l^2 2\pi \int_{-1}^{1} P_l^2(w)\mathrm{d}w = c_l P_l(1).$$

Finally, we use

$$\int_{-1}^{1} P_l^2(w)\mathrm{d}w = \frac{2}{2l+1}, \quad P_l(1) = 1.$$

□

6.8 Harmonic functions and solid harmonics

We say that a function F is *harmonic* if $\Delta F = 0$. For instance, a function depending only on $x + \mathrm{i}y$ or only on $x - \mathrm{i}y$ (that is, iterpreting $\mathbb{R}^2$ as $\mathbb{C}$, analytic or antianalytic) is harmonic.

We say that a function F is homogeneous of degree l if

$$F(\lambda x, \lambda y, \lambda z) = \lambda^l F(x,y,z), \quad \lambda > 0. \tag{6.45}$$

Differentiating in λ we obtain the equivalent condition

$$(x\partial_x + y\partial_y + z\partial_z)F = lF. \tag{6.46}$$

In spherical coordinates the operator on the left hand side is $r\partial_r$. Every function homogeneous of degree l in spherical coordinates can be written as

$$F(r,\theta,\phi) = r^l G(\theta,\phi), \tag{6.47}$$

where G is the restriction of F to $\mathbb{S}^2$.

Theorem 6.6 *If F is harmonic and homogeneous of degree l, then*

$$-\Delta_{\mathbb{S}^2} F = l(l+1)F. \tag{6.48}$$

Proof.

$$\begin{aligned} 0 = \Delta F &= \Big(\partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^2}\Big)F \qquad (6.49)\\ &= \frac{1}{r^2}\Big(r\partial_r(r\partial_r + 1) + \Delta_{\mathbb{S}^2}\Big)F. \qquad (6.50) \end{aligned}$$

□

We say that H is a *solid harmonic of degree* l if it is a harmonic polynomial of degree l. By Thm 6.6, if H is a solid harmonic, then its restriction Y to the sphere is a smooth function satisfying

$$\Delta_{\mathbb{S}^2} Y = -l(l+1)Y, \tag{6.51}$$

or it is a spherical harmonic. One can also show the converse statement:

Theorem 6.7 *Every spherical harmonic is a restriction of a certain solid harmonic to the sphere.*

Here are examples of solid and the corrsponding spherical harmonics:

$$\begin{array}{rcl} 1 = & r^0 & \sim Y_{0,0}, \\ x+\mathrm{i}y = & r(1-w^2)^{\frac12}\mathrm{e}^{\mathrm{i}\phi} & \sim rY_{1,1}, \\ z = & rw & \sim rY_{1,0}, \\ x-\mathrm{i}y = & r(1-w^2)^{\frac12}\mathrm{e}^{-\mathrm{i}\phi} & \sim rY_{1,-1}, \\ (x+\mathrm{i}y)^2 = & r^2(1-w^2)\mathrm{e}^{\mathrm{i}2\phi} & \sim r^2Y_{2,2}, \\ z(x+\mathrm{i}y) = & r^2(1-w^2)^{\frac12}w\mathrm{e}^{\mathrm{i}\phi} & \sim r^2Y_{2,1}, \\ 2z^2-x^2-y^2 = & r^2(3w^2-1) & \sim r^2Y_{2,0}, \\ z(x-\mathrm{i}y) = & r^2(1-w^2)^{\frac12}w\mathrm{e}^{-\mathrm{i}\phi} & \sim r^2Y_{2,-1}, \\ (x-\mathrm{i}y)^2 = & r^2(1-w^2)\mathrm{e}^{-\mathrm{i}2\phi} & \sim r^2Y_{2,-2}. \end{array}$$

6.9 Electrostatic potential

We have

$$\Delta(x^2+y^2+z^2)^{-\frac12} = -4\pi\delta(x)\delta(y)\delta(z).$$

Hence $(x^2+y^2+z^2)^{-\frac12}$ is harmonic on $\mathbb{R}^3\backslash\{(0,0,0)\}$. After a translation it is still harmonic. Hence

$$(x^2+y^2+(z-1)^2)^{-\frac12} \tag{6.52}$$

is harmonic on $\mathbb{R}^3\backslash\{(0,0,1)\}$

Theorem 6.8 *For $|r|<1$ and $-1\leq w=-\cos\theta\leq 1$ we have*

$$(r^2-2r\cos\theta+1)^{-\frac12} = \sum_{l=0}^{\infty} r^l P_l(w). \tag{6.53}$$

Hence,

$$P_l(w) = \frac{1}{l!}\partial_r^l(r^2-2rw+1)^{-\frac12}\Big|_{r=0}. \tag{6.54}$$

Proof. The function $r\mapsto(r^2-2r\cos\theta+1)^{-\frac12}$ has branch points at zeros of $r^2-2r\cos\theta+1$, that is, at $r=w\pm\mathrm{i}\sqrt{1-w^2}$. Therefore, it is analytic in the disc $|r|<1$ and can be expanded in a series in r.

The function (6.53) is spherical coordinates is $(r^2-2r\cos\theta+1)^{-\frac12}$.

$$\begin{aligned} 0 &= \Delta(r^2-2rw+1)^{-\frac12} \\ &= \left(\partial_r^2+\frac{2}{r}\partial_r+\frac{1}{r^2}\left((1-w^2)\partial_w^2-2w\partial_w+\frac{1}{1-w^2}\partial_\phi^2\right)\right)\sum_{l=0}^{\infty} r^l P_l(w) \\ &= \sum_{l=0}^{\infty} r^{l-2}\left(l(l-1)+2l+(1-w^2)\partial_w^2-2w\partial_w\right)P_l(w). \end{aligned}$$

Hence $P_l(w)$ satisfy the lth Legendre equation.

$$\big((1-w^2)\partial_w^2 - 2w\partial_w + l(l+1)\big)\, P_l(w) = 0. \tag{6.55}$$

The formula (6.55) easily implies that $P_l(w)$ are lth degree polynomials. Therefore, $P_l(w)$ are proportional to Legendre polynomials.

We set $w = 1$:

$$(r^2 - 2r + 1)^{-\frac{1}{2}} \;=\; (1-r)^{-1} = \sum_{l=0}^{\infty} r^l = \sum_{l=0}^{\infty} r^l P_l(1).$$

Hence $P_l(w)$ are Legendre polynomials. □

Corollary 6.9 *The electrostatic charge 4π situated at $(0,0,r)$ generates the following potential at the distance R from the center and at the angle $\cos\theta = w$:*

$$(R^2 - 2Rrw + r^2)^{-\frac{1}{2}} \;=\; \begin{cases} \sum\limits_{l=0}^{\infty} r^l R^{-l-1} P_l(w), & R > r; \\ \sum\limits_{l=0}^{\infty} R^l r^{-l-1} P_l(w), & R < r. \end{cases}$$

Proof. We apply (6.54) to

$$(R^2 - 2Rrw + r^2)^{-\frac{1}{2}} = \begin{cases} R^{-1}\Big(1 - 2w\frac{r}{R} + \frac{r^2}{R^2}\Big)^{-\frac{1}{2}}, & r < R; \\ r^{-1}\Big(1 - 2w\frac{R}{r} + \frac{R^2}{r^2}\Big)^{-\frac{1}{2}}, & R < r. \end{cases} \tag{6.56}$$

6.10 Solving second order equations

Consider the equation

$$g(t) = (\partial_t^2 - A^2) f(t), \tag{6.57}$$

where A is a positive operator.

Theorem 6.10 *Depending on the problem, we have the following solutions of (6.58):*

(1) *Given $f(0)$, $f'(0)$:*

$$\begin{aligned} f(t) =& \frac{\mathrm{e}^{tA}}{2A}\Big(Af(0) + f'(0) + \int_0^t \mathrm{e}^{-uA} g(u)\mathrm{d}u\Big) \\ &+ \frac{\mathrm{e}^{-tA}}{2A}\Big(Af(0) - f'(0) - \int_0^t \mathrm{e}^{uA} g(u)\mathrm{d}u\Big). \end{aligned} \tag{6.58}$$

(2) $\lim\limits_{t\to\infty} f(t) = 0$, *given $f(0)$:*

$$f(t) = \mathrm{e}^{-tA} f(0) - \frac{\mathrm{e}^{-tA}}{2A}\int_0^t (\mathrm{e}^{-uA} - \mathrm{e}^{uA}) g(u)\mathrm{d}u + \frac{\mathrm{e}^{tA} - \mathrm{e}^{-tA}}{2A}\int_t^{\infty} \mathrm{e}^{-uA} g(u)\mathrm{d}u; \tag{6.59}$$

(3) $\lim\limits_{t\to\infty} f(t)=0$, *given* $f'(0)$*:*

$$f(t)=-\frac{\mathrm{e}^{-tA}}{A}f'(0)-\frac{\mathrm{e}^{-tA}}{2A}\int_0^t(\mathrm{e}^{uA}+\mathrm{e}^{-uA})g(u)\mathrm{d}u-\frac{\mathrm{e}^{-tA}+\mathrm{e}^{tA}}{2A}\int_t^\infty \mathrm{e}^{-uA}g(u)\mathrm{d}u. \quad (6.60)$$

Proof. We rewrite (6.58) as

$$h=(\partial_t+A)f, \quad (6.61)$$

$$g=(\partial_t-A)h. \quad (6.62)$$

We obtain

$$f(t)=\mathrm{e}^{-tA}f(0)+\int_0^t \mathrm{e}^{-(t-s)A}h(s)\mathrm{d}s, \quad (6.63)$$

$$h(s)=\mathrm{e}^{sA}h(0)+\int_0^s \mathrm{e}^{(s-u)A}g(u)\mathrm{d}u. \quad (6.64)$$

Then we substitute (6.65) into (6.64), which yields (6.59).

Suppose now that there exists $\lim\limits_{t\to\infty} f(t)$. Then the first term of (6.59) has to converge to 0. Therefore,

$$Af(0)+f'(0)+\int_0^\infty \mathrm{e}^{-uA}g(u)\mathrm{d}u=0.$$

To daje (6.60) i (6.61). □

For example, consider the Dirichlet/Neumann problem on the halfspace (t,x_1,x_2), $t>0$. Consider the equation

$$0=\Delta_3 f=\Big(\partial_t^2-\big(\sqrt{-\Delta_2}\big)^2\Big)f, \quad \Delta_2=\partial_1^2+\partial_2^2.$$

The operator $\frac{\exp\left(-t\sqrt{-\Delta_2}\right)}{\sqrt{-\Delta_2}}$ has the integral kernel

$$\frac{\exp\big(-t\sqrt{-\Delta_2}\big)}{\sqrt{-\Delta_2}}(x,y)=\frac{1}{2\pi\sqrt{t^2+(x-y)^2}}. \quad (6.65)$$

This can be obtained as follows:

$$\begin{aligned}&\frac{1}{(2\pi)^2}\int\frac{\mathrm{e}^{\mathrm{i}k(x-y)-|k|t}}{|k|}\mathrm{d}k\\ =&\int_0^\infty \mathrm{d}|k|\int_0^{2\pi}\mathrm{d}\phi \mathrm{e}^{|k|(\mathrm{i}|x-y|\cos\phi-t)}\\ =&\frac{1}{(2\pi)^2}\int_0^{2\pi}\frac{\mathrm{d}\phi}{t-\mathrm{i}|x-y|\cos\phi}.\end{aligned}$$

Then we insert

$$\int_0^{2\pi}\frac{\mathrm{d}\phi}{t-\mathrm{i}a\cos\phi}=\frac{2\pi}{\sqrt{t^2+a^2}}.$$

6.11 Laplace equation on the ball

Consider the Laplace equation on the 3-dimensional unit ball. Write the Laplacian in the coordinates r, w, ϕ. Substitute $r = \mathrm{e}^{-t}$. We obtain $\partial_r = -\mathrm{e}^{t}\partial_t$. Therefore,

$$\Delta = \mathrm{e}^{2t}(\partial_t^2 - \partial_t + \Delta_{\mathbb{S}^2}) = \mathrm{e}^{2t}\big((\partial_t - \tfrac{1}{2})^2 + \Delta_{\mathbb{S}^2} - \tfrac{1}{4}\big). \tag{6.66}$$

Hence

$$\mathrm{e}^{-\frac{5t}{2}}\Delta\mathrm{e}^{\frac{t}{2}} = \partial_t^2 + \Delta_{\mathbb{S}^2} - \tfrac{1}{4} = \partial_t^2 - \Big(\sqrt{-\Delta_{\mathbb{S}^2} + \tfrac{1}{4}}\Big)^2 \tag{6.67}$$

Let us compute the integral kernel of the operator $\frac{\exp\left(-t\sqrt{-\Delta_{\mathbb{S}^2}+\frac{1}{4}}\right)}{\sqrt{-\Delta_{\mathbb{S}^2}+\frac{1}{4}}}$.

We have

$$-\Delta_{\mathbb{S}^2} = \sum_{l=0}^{\infty}\big((l+\tfrac{1}{2})^2 - \tfrac{1}{4}\big)\mathbb{P}_l.$$

Hence,

$$\sum_{l=0}^{\infty}\Big(l + \frac{1}{2}\Big)\mathbb{P}_l = \sqrt{-\Delta_{\mathbb{S}^2} + \tfrac{1}{4}}.$$

After substitution $r = \mathrm{e}^{-t}$, the multipole decomposition leads to

$$\begin{aligned}
\frac{1}{2\pi}\mathrm{e}^{-\frac{t}{2}}(\mathrm{e}^{-2t} - 2\mathrm{e}^{-t}\xi\cdot\eta + 1)^{-\frac{1}{2}} &= \frac{1}{2\pi}\big(2\cosh t - 2\xi\cdot\eta\big)^{-\frac{1}{2}} \\
&= \frac{1}{2\pi}\sum_{l=0}^{\infty}\mathrm{e}^{-(l+\frac{1}{2})t}P_l(\xi\cdot\eta) \qquad (6.68)\\
&= \sum_{l=0}^{\infty}\frac{2\mathrm{e}^{-(l+\frac{1}{2})t}}{2l+1}\mathbb{P}_l(\xi,\eta) \\
&= \frac{\exp\big(-t\sqrt{-\Delta_{\mathbb{S}^2}+\frac{1}{4}}\big)}{\sqrt{-\Delta_{\mathbb{S}^2}+\frac{1}{4}}}(\xi,\eta). \qquad (6.69)
\end{aligned}$$

7 Spherical harmonics in any dimension

7.1 Space $L^2(\mathbb{R}^d)$

Consider the space $L^2(\mathbb{R}^d)$. Here are various unitary operators that act on this space: translations $\mathrm{e}^{-t\partial_{x_i}}$, rotations $\mathrm{e}^{-\psi L_{ij}}$ and scaling $\mathrm{e}^{s(D+\frac{d}{2})}$, where

$$\begin{aligned}
L_{ij} &= x_i\partial_{x_j} - x_j\partial_{x_i}, \\
D: &= x_1\partial_{x_1} + \cdots + x_d\partial_{x_d}.
\end{aligned}$$

7.2 Laplacian

We define the Laplacian:

$$\Delta = \sum_{i=1}^{d} \partial_{x_i}^2.$$

It is easy to see that Δ is invariant wrt translations and rotations:

$$\begin{aligned}
\mathrm{e}^{-t\partial_{x_i}}\Delta &= \Delta\mathrm{e}^{-t\partial_{x_i}}, \\
\mathrm{e}^{-\psi L_{ij}}\Delta &= \Delta\mathrm{e}^{-\psi L_{ij}}.
\end{aligned}$$

7.3 Laplace-Beltrami operator on $\mathbb{S}^{d-1}$

Define

$$L^2 := \sum_{i<j} L_{ij}^2$$

Note that for any ij,

$$\mathrm{e}^{-\psi L_{ij}}L^2 = L^2\mathrm{e}^{-\psi L_{ij}}.$$

Hence the operator L^2 is invariant wrt rotations. It is also invariant wrt scaling and multiplication by r:

$$\begin{aligned}
\mathrm{e}^{-s(D+\frac{d}{2})}L^2 &= L^2\mathrm{e}^{-s(D+\frac{d}{2})}, \\
rL^2 &= L^2 r.
\end{aligned}$$

The operator L^2 is made out of differentiations tangent to the $d-1$-dimensional sphere. It can be viewed as an operator on functions on the unit sphere $\mathbb{S}^{d-1}$. With this interpretation it will be called the Laplace'-Beltrami operator on $\mathbb{S}^{d-1}$, and will be denoted $\Delta_{\mathbb{S}^2}$.

7.4 Spherical coordinates

Suppose that $\Omega = (\omega_1, \dots, \omega_{d-1})$ are coordinates on the sphere.

Adjoining $r := \sqrt{x_1^2 + \cdots + x_d^2}$ to $\Omega = (\omega_1, \dots, \omega_{d-1})$ we obtain coordinates on $\mathbb{R}^d$. (These coordinates can be called "generalized spherical coordinates").'

Theorem 7.1 *We have*

$$\begin{aligned}
D &= r\partial_r, && (7.1)\\
\Delta &= r^{-d+1}\partial_r r^{d-1}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^2} \\
&= \partial_r^2 + \frac{d-1}{r}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^2}. && (7.2)
\end{aligned}$$

Besides, L_{ij} and $\Delta_{\mathbb{S}^2}$ depend only on the coordinates Ω on the sphere.

Proof. We can write

$$D = c_0(r,\Omega)\partial_r + \sum_{j=1}^{d-1} c_j(r,\Omega)\partial_{\omega_j}.$$

We have

$$\begin{aligned} D\sqrt{x_1^2+\cdots+x_d^2} &= \sqrt{x_1^2+\cdots+x_d^2}, \\ D\frac{x_j}{\sqrt{x_1^2+\cdots+x_d^2}} &= 0, \qquad j=1,\dots,d. \end{aligned}$$

The second formula implies $D\omega_j = 0$, $j=1,\dots,d-1$. The first yields $c_0(r,\Omega) = r$. This proves (7.1).

We have

$$L_{ij}^2 = x_i^2\partial_{x_j}^2 + x_j^2\partial_{x_i}^2 - x_ix_j\partial_{x_i}\partial_{x_j} - x_i\partial_{x_i} - x_j\partial_{x_j}.$$

Therefore,

$$\begin{aligned} \sum_{i<j} L_{ij}^2 &= \sum_{i\neq j} x_i^2\partial_{x_j}^2 - \sum_{i\neq j} x_ix_j\partial_{x_i}\partial_{x_j} - (d-1)\sum_i x_i\partial_{x_i} \\ &= \sum_{i,j} x_i^2\partial_{x_j}^2 - \sum_{i,j} x_ix_j\partial_{x_i}\partial_{x_j} - (d-1)\sum_i x_i\partial_{x_i} \\ &= \sum_{i,j} x_i^2\partial_{x_j}^2 - \big(\sum_i x_i\partial_{x_i}\big)^2 - (d-2)\sum_i x_i\partial_{x_i} \\ &= r^2\Delta - D^2 - (d-2)D. \end{aligned}$$

This proves (7.2).

We have $L_{ij}r = rL_{ij}$. Therefore, L_{ij} does not contain a derivative wrt r.

We also have $L_{ij}D = DL_{ij}$. Using $D = r\partial_r$ we see that L_{ij} does not involve r.

The definiton $\Delta_{S^{d-1}}$ involves only L_{ij}. Hence $\Delta_{S^{d-1}}$ does not contain ∂_r nor r. $\square$

7.5 Space $L^2(S^{d-1})$

The unit sphere in $\mathbb{R}^d$ is denoted

$$\mathbb{S}^{d-1} := \{(x_1,\dots,x_d)\in\mathbb{R}^d \ : \ x_1^2+\cdots+x_d^2 = 1\}.$$

$\mathrm{d}\Omega$ stands for the natural measure on $\mathbb{S}^{d-1}$. This measure is invariant wrt rotations and the sphere has the $d-1$-dimensional volume $\frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})}$. The Hilbert space $L^2(\mathbb{S}^{d-1})$ consisits of measurable functions on $\mathbb{S}^{d-1}$ such that

$$\int |f(\Omega)|^2 \mathrm{d}\Omega < \infty.$$

Its scalar product is

$$(f|g) = \int \overline{f(\Omega)}g(\Omega)\mathrm{d}\Omega.$$

The change from the Cartesian to sherical variables ccan be interpreted as the unitary map $U: L^2(\mathbb{R}^d) \to L^2([0,\infty[\times\mathbb{S}^{d-1},\ r^{d-1}\mathrm{d}r\mathrm{d}\Omega)$ defined by

$$(Uf)(r,\Omega) := f(x_1,\dots,x_d).$$

The operator $U\mathrm{e}^{\psi L_{ij}}U^{-1}$ and $U\Delta_{\mathbb{S}^{d-1}}U^{-1}$ act only on the variables Ω. Therefore, they can be interpreted as operators on $L^2(\mathbb{S}^{d-1})$. Abusing slightly the notation, these operators will be denoted simply by $\mathrm{e}^{\psi L_{ij}}$ and $\Delta_{\mathbb{S}^{d-1}}$. The operators $\mathrm{e}^{\psi \tilde{L}_{ij}}$ are unitary on $L^2(\mathbb{S}^{d-1}\mathrm{d}\Omega)$. The operator $\Delta_{\mathbb{S}^{d-1}}$ is self-adjoint on $L^2(\mathbb{S}^{d-1}\mathrm{d}\Omega)$ and is called the Laplace-Beltrami operator on the unit sphere. We would like to diagonalize $\Delta_{\mathbb{S}^{d-1}}$.

7.6 Multivariable polynomials

A polynomial depending on the variables $x_1,\dots,x_d$ is a finite linear compbination of expressions of the form

$$x_1^{k_1}\cdots x_d^{k_d}.$$

Thus, every polynomial has the form

$$P(x_1,\cdots x_d) = \sum_{k_1,\dots,k_d} P_{k_1,\dots k_d} x_1^{k_1}\cdots x_d^{k_d}.$$

The degree of a polynomial P is defined as

$$\mathrm{deg}P := \max\{k_1+\cdots+k_d \ : \ P_{k_1,\dots,k_d}\neq 0\}.$$

7.7 Homogeneous polynomials

We say that a polynomial P is homogeneous of degree l if

$$P(\lambda x_1,\cdots \lambda x_d) = \lambda^l P(x_1,\cdots x_d).$$

In other words,

$$P(x_1,\cdots x_d) = \sum_{k_1+\cdots+k_d=l} P_{k_1,\dots,k_d} x_1^{k_1}\cdots x_d^{k_d}.$$

Here is an equivalent condition:

$$r\partial_r P = lP. \tag{7.3}$$

Let Pol^l denote the space of polynomials homogeneous of degree l.

Theorem 7.2 *The dimension of the space of polynomials of degree l of d variables is*

$$\dim \mathrm{Pol}^l = \left(\begin{array}{c} d+l-1 \\ d-1 \end{array}\right) = \frac{(d+l-1)!}{(d-1)!l!}. \tag{7.4}$$

Proof. Consider a row of $d+l-1$ white balls. We paint black $d-1$ balls. We obtain d smaller rows of white balls. In the jth row there are k_j balls, altogether $k_1+\cdots+k_d = d+l-1-(d-1) = l$. The number of such configurations is the same as the number of $d-1$ element combinations in an $l+d-1$-element set, that is, (7.4). $\square$

7.8 Harmonic polynomials

We say that a polynomial H is harmonic if

$$\Delta H = 0.$$

Let Har^l denote the space of harmonic polynomials homogeneous of degree l. (The second implicit parameter is the dimension of the space d).

Harmonic polynomials homogeneous of degree l are sometimes called solid harmonics of degree l.

Theorem 7.3 (1) $\dim \mathrm{Har}^l = \dim \mathrm{Pol}^l - \dim \mathrm{Pol}^{l-2} = \frac{(2l+d-2)(d+l-3)!}{(d-2)!l!}$.

(2) $\mathrm{Pol}^l = \mathrm{Har}^l \oplus r^2\mathrm{Pol}^{l-2}$.

(3) *The operator* Δ *is injective on* $r^2\mathrm{Pol}^{l-2}$.

Proof. Let $P \in r^2\mathrm{Pol}^{l-2}$ and $\Delta P = 0$. We can write

$$P = r^{2k}P_{l-2k},$$

where $P_{l-2k} \in \mathrm{Pol}^{l-2k}$ is not divisible by r^2 and $k \geq 1$.

$$\begin{aligned}
\Delta r^{2k}P_{l-2k} &= (\Delta r^{2k})P_{l-2k} + 2(\nabla r^{2k})\nabla P_{l-2k} + r^{2k}\Delta P_{l-2k} \\
&= 2k(2k-2+d)r^{2k-2}P_{l-2k} + 4kr^{2k-2}r\partial_r P_{l-2k} + r^{2k}\Delta P_{l-2k} \\
&= 2k\big(-2k-2+d+2l\big)r^{2k-2}P_{l-2k} + r^{2k}\Delta P_{l-2k}.
\end{aligned}$$

We have $2k(-2k-2+d+2l) > 0$. Hence P_{l-2k} is divisible by r^2, which is a contradiction and proves (3).

Consider the linear operator $\Delta_l : \mathrm{Pol}^l \to \mathrm{Pol}^{l-2}$. Using (3) we obtain

$$\dim \mathrm{Pol}^{l-2} \geq \dim \mathrm{Ran}\Delta_l \geq \dim r^2\mathrm{Pol}^{l-2} = \mathrm{Pol}^{l-2}. \tag{7.5}$$

Hence $\dim \mathrm{Pol}^{l-2} = \dim \mathrm{Ran}\Delta_l$. But

$$\dim \mathrm{Pol}^l = \dim \mathrm{Ran}\Delta^l + \dim \mathrm{Ker}\Delta^l \tag{7.6}$$

and $\mathrm{Ker}\Delta_l = \mathrm{Har}^l$. This proves (1). Finally, (1) and (3) implies (2). □

Here are examples of solid harmonics:

$d = 2$. For $m \geq 1$ in the Cartesian and polar coordinates:

$$(x \pm \mathrm{i}y)^m = r^m \mathrm{e}^{\pm \mathrm{i}m\phi}.$$

$\dim \mathrm{Har}^0 = 1$, $\dim \mathrm{Har}^l = 2$, $l \geq 1$.

$d = 3$. Solid harmonics for $l \geq 1$ in Cartesian and spherical coordinates:

$$(x\sin\psi - y\cos\psi \pm \mathrm{i}z)^l = r^l(\sin\theta\sin(\phi-\psi) \pm \mathrm{i}\cos\theta)^l$$

$\dim \mathrm{Har}^l = 2l + 1$.

7.9 Spherical harmonics

We say that a funtion $Y : \mathbb{S}^{d-1} \to \mathbb{C}$ is a spherical harmonic of degree l, if there exists a solid harmonic H of degree l such that Y is a restriction of H to $\mathbb{S}^{d-1}$. An equivalent condition:

$$(x_1^2 + \cdots x_d^2)^{\frac{l}{2}} Y \left(\frac{x_1, \dots x_d}{\sqrt{x_1^2 + \cdots x_d^2}} \right)$$

is a harmonic polynomial.

Here are examples of spherical harmonics:

$d = 2$

$$\mathrm{e}^{\pm \mathrm{i} m \phi}.$$

$d = 3$

$$(\sin\theta \sin(\phi + \psi) \pm \mathrm{i}\cos\theta)^l.$$

Lemma 7.4 *Let $P \in \mathrm{Pol}^l$. Then there exist $H_{l-2k} \in \mathrm{Har}^{l-2k}$, $k = 0, \dots [l/2]$, such that*

$$P\Big|_{\mathbb{S}^{d-1}} = \sum_{k=0}^{[l/2]} H_{l-2k}\Big|_{\mathbb{S}^{d-1}}. \tag{7.7}$$

Proof. We use induction wrt l.

We have

$$\mathrm{Pol}^0 = \mathrm{Har}^0, \quad \mathrm{Pol}^1 = \mathrm{Har}^1.$$

Hence the lemma is obvious for $l = 0, 1$.

Suppose that the lemma is true for l replaced with $l - 2$. By Thm 7.3, we have

$$P = r^2 P_{l-2} + Q_l, \quad P_{l-2} \in \mathrm{Pol}^{l-2}, \quad Q_l \in \mathrm{Har}^l. \tag{7.8}$$

By the induction assumption,

$$P_{l-2}\Big|_{\mathbb{S}^{d-1}} = \sum_{k=1}^{[l/2]} Q_{l-2k}\Big|_{\mathbb{S}^{d-1}}, \quad Q_{l-2k} \in \mathrm{Har}^{l-2k}. \tag{7.9}$$

But on $\mathbb{S}^{d-1}$ we have $r^2 = 1$. Therefore, (7.8) and (7.9) imply (7.7). □

Theorem 7.5 *Let Y_l be a spherical harmonic of degree l. Then*

$$\Delta_{\mathbb{S}^{d-1}} Y_l = -l(l + d - 2) Y_l.$$

Proof.

$$
\begin{aligned}
0 = \Delta r^l Y_l &= \left(r^{-d+1}\partial_r r^{d-1}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}}\right) r^l Y_l \\
&= l(l+d-2) r^{l-2} Y_l + r^{l-2}\Delta_{\mathbb{S}^{d-1}} Y_l.
\end{aligned}
$$

□

Spherical harmonics of degree l form a subspace of $L^2(\mathbb{S}^{d-1})$ denoted $\mathcal{H}_l$.

Theorem 7.6 (1) *$\mathcal{H}_l$ is the subspace of eigenfunctions of the operator $-\Delta_{\mathbb{S}^{d-1}}$ on $L^2(\mathbb{S}^{d-1})$ with eigenvalue $l(l+d-2)$.*

(2) *$\mathcal{H}_l$ are orthogonal to one another for disctinct l.*

(3) *Linear combinations of elements of $\mathcal{H}_l$ are dense in $L^2(\mathbb{S}^{d-1})$.*

(4) *Rotation operators $\mathrm{e}^{\psi L_{ij}}$ preserve $\mathcal{H}_l$.*

Proof. (2) follows from (1) and from the self-adjointness of $\Delta_{\mathbb{S}^{d-1}}$ on $L^2(\mathbb{S}^{d-1})$.

Lemma 7.4 shows that harmonic polynomials restricted to $\mathbb{S}^{d-1}$ coincide with all polynomials restricted to $\mathbb{S}d-1$.pokazuje, że wielomiany harmoniczne obcięte do sfery. Then we use the Stone-Weierstrass Theorem, which implies that polynomials are dense in continuous functions on $\mathbb{S}^{d-1}$ in the supremum norm. Continuous functions are dense in $L^2(\mathbb{S}^{d-1})$. This shows (3).

(4) follows from $\mathrm{e}^{\psi L_{ij}}\Delta_{\mathbb{S}^{d-1}} = \Delta_{\mathbb{S}^{d-1}}\mathrm{e}^{\psi L_{ij}}$. □

(2) and (3) cn be together expressed by the identity $L^2(\mathbb{S}^{d-1}) = \bigoplus\limits_{l=0}^{\infty}\mathcal{H}_l$.

7.10 Gegenbauer polynomials

Gegenbauer polynomials are defined with the help of the following generating function:

$$
(1-2wr+r^2)^{-\lambda} = \sum_{n=0}^{\infty} r^n C_n^\lambda(w), \quad |r|<1. \tag{7.10}
$$

Hence,

$$
C_n^\lambda(w) = \frac{1}{n!}\partial_r^n (r^2-2wr+1)^{-\lambda}\Big|_{r=0}.
$$

We have

$$
(r^2-2r+1)^{-\lambda} = (r-1)^{-2\lambda} = \sum_{n=0}^{\infty}\frac{(2\lambda)_n}{n!}r^n.
$$

Hence,

$$
C_n^\lambda(1) = (2\lambda)_n.
$$

Substituting $R=\frac{1}{r}$, (7.10) can be rewritten as

$$
(1-2wR+R^2)^{-\lambda} = \sum_{n=0}^{\infty} R^{-2\lambda-n} C_n^\lambda(w), \quad |R|>1.
$$

Proposition 7.7

$$\Big((1-w^2)\partial_w^2-(1+2\lambda)w\partial_w+n(n+2\lambda)\Big)C_n^\lambda(w)=0.$$

Proof. Clearly,

$$\begin{aligned}\Big(\partial_x^2+\partial_y^2\Big)(x^2+y^2)^{-\lambda} &= (2\lambda)^2(x^2+y^2)^{-\lambda-1},\\ \frac{1}{y}\partial_y(x^2+y^2)^{-\lambda} &= -2\lambda(x^2+y^2)^{-\lambda-1}.\end{aligned}$$

Hence,,

$$\Big(\partial_x^2+\partial_y^2+\frac{2\lambda}{y}\partial_y\Big)(x^2+y^2)^{-\lambda} = 0.$$

Therefore,,

$$\Big(\partial_x^2+\partial_y^2+\frac{2\lambda}{y}\partial_y\Big)\big((x-1)^2+y^2\big)^{-\lambda} = 0. \tag{7.11}$$

Introduce polar coordinates:

$$\begin{aligned}x=rw,&\qquad y=r\sqrt{1-w^2},\\ r=\sqrt{x^2+y^2},&\qquad w=\frac{x}{\sqrt{x^2+y^2}}.\end{aligned}$$

We have then

$$\begin{aligned}\partial_x &= w\partial_r+\frac{1-w^2}{r}\partial_w,\\ \partial_y &= \sqrt{1-w^2}\partial_r-\frac{w\sqrt{1-w^2}}{r}\partial_w.\end{aligned}$$

$$\begin{aligned}\partial_x^2+\partial_y^2 &= \partial_r^2+\frac{1}{r}\partial_r+\frac{1}{r^2}\Big((1-w^2)\partial_w^2-w\partial_w\Big),\\ \frac{1}{y}\partial_y &= \frac{1}{r}\partial_r-\frac{w}{r^2}\partial_w.\end{aligned}$$

(7.11) can be rewritten as

$$\Big(\partial_r^2+\frac{(1+2\lambda)}{r}\partial_r+\frac{1}{r^2}\big((1-w^2)\partial_w^2-(1+2\lambda)w\partial_w\big)\Big)(r^2-2wr+1)^{-\lambda}=0. \tag{7.12}$$

□

Thus Gegenbauer polynomials satisfy the same equation as ultraspherical (Jacobi) polynomials with $\alpha=\lambda-\frac{1}{2}$. Hence C_n^λ is proportional to $P_n^{\lambda-\frac12,\lambda-\frac12}$. Comparing the value at 1 we obtain

$$C_n^\lambda(w)=\frac{(2\lambda)_n}{(\lambda+\frac12)_n}P_n^{\lambda-\frac12,\lambda-\frac12}(w).$$

Comparing the generating functions we obtain the relations between Gegenbauer and Chebyshev polynomials:

$$\begin{aligned}T_n(w) &= \frac{1}{2}\partial_\lambda C_n^\lambda(w)\Big|_{\lambda=0},\\ U_n(w) &= C_n^1(w).\end{aligned}$$

7.11 Electrostatic potential in higher dimensions

The Laplacian in dimension d on radial functions is

$$\partial_r^2 + \frac{d-1}{r}\partial_r. \tag{7.13}$$

Therefore,

$$r^{-2\lambda} = (x_1^2 + \cdots + x_d^2)^{-\lambda}$$

for $\lambda = \frac{d}{2} - 1$ is harmonic on $\mathbb{R}^d$ outside zero.

Similarly, the function

$$\big(x_1^2 + \cdots + x_{d-1}^2 + (x_d - 1)^2\big)^{-\lambda} \tag{7.14}$$

is harmonic outside of $(0, \dots, 0, 1)$. Introducing $w := \frac{x_d}{r}$ we can rewrite (7.14) as

$$(1 + r^2 - 2wr)^{-\lambda}. \tag{7.15}$$

For functions depending only on r, w, the Laplacian is

$$\partial_r^2 + \frac{d-1}{r}\partial_r + \frac{1}{r^2}\big((1-w^2)\partial_w^2 - (d-1)w\partial_w\big).$$

This operator annihilates (7.15), which yieds an alternative proof of (7.12) (which unfortunately works only for $\lambda = \frac{1}{2}, 1, \dots$).