4. Hermite and Laguerre polynomials

4.1 Hermite polynomials from a generating function

We will see that Hermite polynomials are solutions to the radial part of the Schrodinger Equation for the simple harmonic oscillator.

Learning outcome: Derive Hermite’s equation and the Hermite recurrence relations from the generating function.

Just like Legendre polynomials and Bessel functions, we may define Hermite polynomials $H_n(x)$ via a generating function.

$$g(x, t) = e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} \frac{H_n(x) t^n}{n!}$$

We could, of course, use this to derive the individual polynomials, but this is very tedious. It is better to derive recurrence relations.
\[ g(x, t) = e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \]

Differentiate with respect to \( t \):

\[ \frac{\partial}{\partial t} g(x, t) = (-2t + 2x) e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^{n-1}}{n!} \]

Expand the terms, and put the generating function in again:

\[ -2 \sum_{n=0}^{\infty} H_n(x) \frac{t^{n+1}}{n!} + 2x \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} = \sum_{n=1}^{\infty} H_n(x) \frac{t^{n-1}}{(n-1)!} \]

Relabel:

\[ -2 \sum_{n=1}^{\infty} nH_{n-1}(x) \frac{t^n}{n!} + 2x \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} = \sum_{n=0}^{\infty} H_{n+1}(x) \frac{t^n}{n!} \]

Equating coefficients of \( t^n \):

\[ \Rightarrow \quad H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (n \geq 1) \]
\[ g(x, t) = e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \]

Differentiate with respect to \( x \):

\[ \frac{\partial}{\partial x} g(x, t) = 2t e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} H'_n(x) \frac{t^n}{n!} \]

Stick in \( g \):

\[ 2 \sum_{n=0}^{\infty} H_n(x) \frac{t^{n+1}}{n!} = \sum_{n=1}^{\infty} H'_n(x) \frac{t^n}{n!} \]

Relabel:

\[ 2 \sum_{n=1}^{\infty} H_{n-1}(x) \frac{t^n}{(n-1)!} = \sum_{n=1}^{\infty} H'_n(x) \frac{t^n}{n!} \]

Equating coefficients of \( t^n \):

\[ \Rightarrow \quad H'_n(x) = 2n H_{n-1}(x) \quad (n \geq 1) \]
We can use these recurrence relations to derive the Hermite differential equation (much easier than Legendre’s!).

\[
\begin{align*}
H_{n+1}(x) &= 2xH_n(x) - 2nH_{n-1}(x) \\
H'_n(x) &= 2nH_{n-1}(x)
\end{align*}
\]

\[\Rightarrow \ H_{n+1}(x) = 2xH_n(x) - H'_n(x)\]

Differentiate with respect to \(x\):

\[
H'_{n+1}(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x)
\]

\[2(n + 1)H_n(x) = 2H_n(x) + 2xH'_n(x) - H''_n(x)\]

\[\Rightarrow \ H''_n(x) - 2xH'_n(x) + 2nH_n(x) = 0\]

This is **Hermite’s equation**.
Learning outcome: Use a generating function and recurrence relations to find the first few Hermite polynomials.

Generating function: \( \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} = e^{-t^2 + 2tx} \)

\[ \Rightarrow H_0(x) + H_1(x)t + O(t^2) = 1 - t^2 + 2tx + O(t^2) \Rightarrow \begin{cases} t^0: & \Rightarrow H_0(x) = 1 \\ t^1: & \Rightarrow H_1(x) = 2x \end{cases} \]

Now use the recurrence relation,

\[ H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \]

\[ H_2(x) = 2xH_1(x) - 1 \times 2H_0(x) = 4x^2 - 2 \]

\[ H_3(x) = 2xH_2(x) - 2 \times 2H_1(x) = 8x^3 - 4x - 8x = 8x^3 - 12x \]

\[ H_4(x) = 2xH_3(x) - 3 \times 2H_2(x) = 16x^4 - 24x^2 - (24x^2 - 12) = 16x^4 - 48x^2 + 12 \]
4.2 Properties of Hermite polynomials

Symmetry about $x=0$:

$$g(-x, -t) = e^{-(t)^2 + 2(-t)(-x)} = e^{-t^2 + 2tx} = g(x, t)$$

$$\Rightarrow \sum_{n=0}^{\infty} H_n(-x) \frac{(-t)^n}{n!} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}$$

$$\Rightarrow H_n(-x) = (-1)^n H_n(x)$$

(just like for Legendre polynomials)

There also exists a specific series form:

$$H_n(x) = \sum_{m=0}^{n/2} (-1)^m (2x)^{n-2m} \frac{n!}{(n-2m)!m!}$$

Exercise: Use this series to verify the first few Hermite polynomials.
Exercise:

Writing \( g(x, t) = e^{x^2} e^{-(t-x)^2} \) show that

\[
H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left( e^{-x^2} \right)
\]

This is Rodrigues’ equation for Hermite polynomials.

\[
\text{Hint: work out } \left. \frac{\partial^n g}{\partial t^n} \right|_{t=0} \text{ and observe that } \frac{\partial}{\partial t} e^{-(t-x)^2} = -\frac{\partial}{\partial x} e^{-(t-x)^2}
\]
Learning outcome: Write down the Hermite polynomial orthogonality condition.

Starting from Hermite’s equation: \( H''_n(x) - 2x H'_n(x) + 2n H_n(x) = 0 \)

\[ \Rightarrow \frac{d}{dx} \left( e^{-x^2} \frac{d}{dx} H_n(x) \right) + 2n e^{-x^2} H_n(x) = 0 \]

we proceed much the same way as we did for Legendre polynomials.

\[ \Rightarrow H_m(x) \frac{d}{dx} \left[ e^{-x^2} \frac{d}{dx} H_n(x) \right] - H_n(x) \frac{d}{dx} \left[ e^{-x^2} \frac{d}{dx} H_m(x) \right] \]

\[ = -H_m(x) 2n e^{-x^2} H_n(x) + H_n(x) 2m e^{-x^2} H_m(x) \]

Integrate this over \( x \) from \(-\infty\) to \( \infty \), integrating the left-hand-side by parts.

\[ \int_{-\infty}^{\infty} H_m(x) \frac{d}{dx} \left[ e^{-x^2} \frac{d}{dx} H_n(x) \right] dx = \left[ H_m(x) e^{-x^2} \frac{d}{dx} H_n(x) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \left[ \frac{d}{dx} H_m(x) \right] e^{-x^2} \frac{d}{dx} H_n(x) dx \]

\[ \Rightarrow 2(m - n) \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 0 \]
We say that Hermite polynomials are orthogonal on the interval $[-\infty, \infty]$ with a weighting $e^{-x^2}$

$$\int_{-\infty}^{\infty} g^2(x, t) e^{-x^2} \, dx = \int_{-\infty}^{\infty} e^{-2t^2 + 4tx - x^2} \, dx = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{t^{n+m}}{n! m!} \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} \, dx$$

$$\int_{-\infty}^{\infty} e^{-(x-2t)^2} e^{2t^2} \, dx = e^{2t^2} \int_{-\infty}^{\infty} e^{-x^2} \, dx = e^{2t^2} \sqrt{\pi}$$

$$= \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n}{n!} t^{2n}$$

$$\left[ \int_{-\infty}^{\infty} e^{-x^2} \, dx \right]^2 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \, e^{-x^2 - y^2}$$

$$= \int_{0}^{2\pi} d\theta \int_{0}^{\infty} dr \, r e^{-r^2} = 2\pi \left[ \frac{-1}{2} e^{-r^2} \right]_{0}^{\infty} = \pi$$

Equating powers of $t^{2n}$ gives

$$\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} \, dx = 2^n \sqrt{\pi n!}$$

$$\Rightarrow \quad \int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} \, dx = 2^n \sqrt{\pi n!} \delta_{nm}$$
Exercise: For a continuous function, I can write $f(x) = \sum_{n=0}^{\infty} c_n H_n(x)$. Show that

$$c_n = \frac{1}{2^n \sqrt{\pi} n!} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2} \, dx$$

Sometimes people remove the weighting by redefining the function: $\varphi_n(x) \equiv e^{-x^2/2} H_n(x)$

$$\Rightarrow \int_{-\infty}^{\infty} \varphi_n(x) \varphi_m(x) \, dx = 2^n \sqrt{\pi} n! \delta_{nm}$$

Now this looks like a “traditional” orthogonality relation.

$$H_n(x) = e^{x^2/2} \varphi_n(x) \quad \Rightarrow \quad H'_n(x) = x e^{x^2/2} \varphi_n(x) + e^{x^2/2} \varphi'_n(x)$$
$$\Rightarrow \quad H''_n(x) = e^{x^2/2} \varphi''_n(x) + 2x e^{x^2/2} \varphi'_n(x) + (1+x^2) \varphi_n(x)$$

Then Hermite’s equation $H''_n(x) - 2x H'_n(x) + 2n H_n(x) = 0$ becomes

$$\varphi''_n(x) + (1 - x^2 + 2n) \varphi_n(x) = 0$$
4.3 Hermite polynomials and the Quantum Harmonic Oscillator

Learning Outcome: Solve the quantum harmonic oscillator in terms of Hermite polynomials.

Recall our earlier discussion of the time-independent Schrödinger equation. That was in 3-dimensions, but here I will simplify to one dimension again,

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E \psi(x),\]

where \(m\) is the particle mass, and \(E\) is its energy.

For the simple harmonic oscillator, \(V(x) = \frac{1}{2}m\omega^2x^2\), so the equation becomes

\[\psi''(x) + \left( -\frac{m^2\omega^2}{\hbar^2}x^2 + \frac{2mE}{\hbar^2} \right) \psi(x) = 0\]

Notice that this looks awfully like the equation we just had on the previous slide:

\[\varphi''_n(x) + (1 - x^2 + 2n) \varphi_n(x) = 0\]

Our reweighted Hermite polynomials are solutions of the Quantum Harmonic Oscillator!
Let’s write $y = ax$ with $a = \sqrt{\frac{m\omega}{\hbar}}$ so we get

$$\frac{d^2}{dy^2} \psi \left( \frac{y}{a} \right) + \left( -y^2 + \frac{2mE}{\hbar^2 a^2} \right) \psi \left( \frac{y}{a} \right) = 0$$

Comparing the two equations, we see that we have solutions,

$$\psi_n(x) = \sqrt{\frac{a}{2^n \sqrt{\pi n!}}} e^{-a^2 x^2 / 2} H_n(ax)$$

where the normalization constant in front ensures that $\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, dx = 1$, and,

the energy is given by the equation

$$\frac{2mE}{\hbar^2 a^2} = 1 + 2n \quad \Rightarrow \quad \frac{2E}{\hbar \omega} = 1 + 2n \quad \Rightarrow \quad E = \hbar \omega \left( n + \frac{1}{2} \right)$$

Have you seen this somewhere before?
You probably solved this elsewhere using ladder operators. This works (in part) because of the Hermite recurrence relation \( H_n'(x) = 2nH_{n-1}(x) \).

Writing \( \varphi_n(x) = \sqrt{\frac{1}{2^n \sqrt{\pi n!}}} e^{-x^2/2} H_n(x) \) for simplicity (ie. set \( a=1 \) for now)

Then \[
\frac{1}{\sqrt{2}} \left( x + \frac{d}{dx} \right) \varphi_n(x) = \sqrt{\frac{1}{2^{n+1} \sqrt{\pi n!}}} \left( x + \frac{d}{dx} \right) e^{-x^2/2} H_n(x)
\]

\[
= \sqrt{\frac{1}{2^{n+1} \sqrt{\pi n!}}} \left( xe^{-x^2/2} H_n(x) - xe^{-x^2/2} H_n(x) + e^{-x^2/2} H_n'(x) \right)
\]

\[
= \sqrt{\frac{1}{2^{n+1} \sqrt{\pi n!}}} \left( e^{-x^2/2} 2n H_{n-1}(x) \right) = \sqrt{\frac{n}{2^{n-1} \sqrt{\pi (n-1)!}}} \left( e^{-x^2/2} H_{n-1}(x) \right)
\]

\[
= \sqrt{n} \varphi_{n-1}(x)
\]

This is a **lowering operator**.

**Exercise:** Use recurrence relations to show that the operator \( \frac{1}{\sqrt{2}} \left( x - \frac{d}{dx} \right) \) is a raising operator. Can you show it using the Rodrigues’ equation?
But why is the quantum harmonic oscillator quantized?

We have seen why \( E = \hbar \omega (n + \frac{1}{2}) \), and how to move from one energy state to another using ladder operators, but we still have no reason for why \( n \) must be an integer!

Indeed, Hermite’s equation \( H''_n(x) - 2x H'_n(x) + 2n H_n(x) = 0 \) does have solutions for non-integer values of \( n \).

Plugging \( H_n(x) = \sum_{k=0}^{\infty} c_k x^k \) into the equation, one finds a solution

\[
H_n(x) = c_0 \left[ 1 + \frac{2(-n)}{2!} x^2 + \frac{2^2(-n)(2-n)}{4!} x^4 + \ldots \right] \\
+ c_1 \left[ x + \frac{2(1-n)}{3!} x^3 + \frac{2^2(1-n)(3-n)}{5!} x^5 + \ldots \right]
\]

which is valid for non-integer \( n \). (This is known as a Hermite “function”.)

For integer \( n \), this solution (or to be more precise, half of it) will truncate to give Hermite polynomials.

For non-integer \( n \), it does not truncate and one can show that the terms grow like \( x^n e^{x^2/2} \). These solutions do not satisfy the boundary condition \( \psi(x) \to 0 \) as \( x \to \infty \), so must be discarded and the harmonic oscillator is quantized.
4.4 Laguerre polynomials and the hydrogen atom

Learning outcome: Understand the importance of Laguerre polynomials to the solution of Schrodinger’s equation for the hydrogen atom.

Generating function:

\[ g(x, t) = e^{-xt/(1-t)} = \sum_{n=0}^{\infty} L_n(x)t^n \]

Exercise: Starting from the generating function, prove the two recurrence relations

\[ (n + 1)L_{n+1}(x) = (2n + 1 - x)L_n(x) - nL_{n-1}(x) \]
\[ xL_n'(x) = nL_n(x) - nL_{n-1}(x) \]

Also, show \( L_n(0) = 1 \) and find expressions for the first 4 polynomials.
Following a similar method to that used for Legendre and Hermite polynomials, we can show that the Laguerre polynomials are orthogonal over the interval \([0, \infty]\) with a weighting \(e^{-x}\), i.e.

\[
\int_{0}^{\infty} L_n(x)L_m(x)e^{-x}dx = \delta_{nm}
\]

They satisfy the **Laguerre equation**:

\[
xL_n''(x) + (1 - x)L_n'(x) + nL_n(x) = 0
\]

and have a Rodrigues’ formula

\[
L_n(x) = \frac{e^x}{n!} \frac{d^n}{dx^n} \left( x^n e^{-x} \right)
\]

(These results can be proven using similar methods to those used earlier for Legendre and Hermite polynomials. If you are feeling assiduous feel free to do these as an exercise.)
**Associated Laguerre polynomials** are obtained by differentiating “regular” Laguerre polynomials (just as for Legendre).

\[ L_n^k(x) = (-1)^n \frac{d^k}{dx^k} L_{n+k}(x) \]

**Exercise:** Show that \( L_n^k(x) \) are solutions to the associated Laguerre equation

\[
x L_n''(x) + (k + 1 - x) L_n'(x) + n L_n(x) = 0
\]

These are also orthogonal with

\[
\int_0^\infty L_n^k(x) L_m^k(x) x^k e^{-x} dx = \frac{(n + k)!}{n!} \delta_{nm}
\]
Recall our investigation of the Schrödinger equation in spherical coordinates with \( V = V(r) \).

\[
-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V \psi(r) = E \psi(r)
\]

Separating \( \psi(r) = R(r)Y_{lm}^m(\theta, \phi) \) resulted in spherical harmonics

\[
Y_{lm}^m(\theta, \phi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} e^{im\phi} P_l^m(\cos \theta)
\]

and a radial equation

\[
\frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] - \frac{2m}{\hbar^2} (V(r) - E) r^2 R(r) - l(l+1)R(r) = 0
\]

For the hydrogen atom (that is, with \( \psi(r) \) the wavefunction for an electron orbiting a proton), the potential is the Coulomb potential,

\[
V(r) = \frac{-e^2}{4\pi \varepsilon_0 r}
\]
To make the maths a wee bit cleaner, let’s make the following redefinitions:

\[ \rho = \alpha r, \quad \alpha = \sqrt{-\frac{8mE}{\hbar^2}}, \quad \lambda = \frac{me^2}{2\pi\epsilon_0\alpha\hbar^2}, \quad \chi(\rho) = R(r), \quad \text{with } E < 0 \]

(we regard \( E=0 \) at \( \infty \))

Then

\[
\frac{d}{dr} \left[ r^2 \frac{dR(r)}{dr} \right] - \frac{2m}{\hbar^2} \left( \frac{-e^2}{4\pi\epsilon_0 r} - E \right) r^2 R(r) - l(l+1)R(r) = 0
\]

becomes

\[
\frac{d}{d\rho} \left[ \rho^2 \frac{d\chi(\rho)}{d\rho} \right] + \left( \lambda \rho - \frac{1}{4} \rho^2 - l(l+1) \right) \chi(\rho) = 0
\]

which has solutions containing associated Laguerre polynomials,

\[
\chi(\rho) = e^{-\rho/2} \rho^l L_{\lambda-l-1}^{2l+1}(\rho)
\]
**Exercise:** Plug the above result into the radial equation to recover the associated Laguerre equation for $L(\rho)$.

Just as for the Hermite equation, solutions exist for non-integer $\lambda-l-1$ but these diverge as $r\to\infty$ and must be discarded. The boundary conditions quantize the energy of the Hydrogen atom.

Fixing $\lambda$ to be an integer $n$,

$$E_n = -\frac{\alpha^2 \hbar^2}{8m} = - \frac{e^2}{4\pi\varepsilon_0} \frac{1}{2a_0} \frac{1}{n^2}$$

where $a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2} = \frac{2}{n\alpha}$ is the Bohr radius.

Also, hydrogen wavefunctions are,

$$\psi_{nlm}(r, \theta, \phi) = N_{nlm} e^{-\alpha r/2} (\alpha r)^l L_{n-l-1}^{2l+1} (\alpha r) Y_l^m(\theta, \phi)$$

where $N_{nlm}$ is a normalization coefficient.
To find the normalization coefficient we need

$$
\int_0^{2\pi} \int_0^\pi \int_0^\infty |\psi_{nlm}(r, \theta, \phi)|^2 r^2 \sin \theta \, dr \, d\theta \, d\phi = \alpha^{-3} \int_0^\infty [\chi(\rho)]^2 \rho^2 d\rho
$$

$$
= N^2_{nlm} \frac{1}{\alpha^3} \int_0^\infty e^{-\rho} \rho^{2l+2} L_{n-l-1}^{2l+1}(\rho) L_{n-l-1}^{2l+1}(\rho) \, d\rho = N^2_{nlm} \frac{2n}{\alpha^3} \frac{(n+l)!}{(n-l-1)!} = 1
$$

Notice the $2n$ here. This is because we don’t quite have the orthogonality condition for the associated Laguerre polynomials we had before - we have an extra power of $\rho$. This result is most easily proven with a recurrence relation,

$$
\rho L_n^k = (2n+k+1)L_n^k - (n+k)L_{n-1}^k - (n+1)L_{n+1}^k
$$

Finally, the electron wavefunction in the hydrogen atom is

$$
\psi_{nlm}(r, \theta, \phi) = \left[ \frac{\alpha^3 (n-l-1)!}{2n (n+l)!} \right]^{1/2} (\alpha r)^l e^{-\alpha r/2} L_{n-l-1}^{2l+1} (\alpha r) Y_l^m(\theta, \phi)
$$