7701 Lecture 32 and Background

**Sturm-Liouville Introduction**

What are Sturm-Liouville problems?

Start with probably the simplest example, the familiar Helmholtz equation on $x \in [0, L]$ (or $0 \leq x \leq L$):

$$\frac{d^2y}{dx^2} + k^2 y = 0$$

Physical situation dictates boundary conditions:

i) Vibrating string fixed at ends

$$y(0) = 0, \quad y(L) = 0$$

ii) Pressure (sound) wave in pipe closed at one end

$$y(0) = 0, \quad y'(L) = 0$$

[Aside: which is the open end?]

More general: a mix of conditions on $y$ and $y'$:

$$\left( \text{or } y(x) \right)' \left. \right|_{x=L} = 0$$

(Not is, $y(x)$ satisfies equation and boundary condition)

Features:

- Only certain values of $k$ work $\Rightarrow$ eigenvalue problem
- Corresponding eigenfunctions
  - Eq. i) $y_n(x) = A_n \sin k_n x \Rightarrow k_n L = n \pi \Rightarrow k_n = \frac{n \pi}{L}$
- We can choose $A_n$ so normalized, they are also orthogonal

$$\Rightarrow \int_0^L y_m(x) y_n(x) \, dx = \delta_{mn} \quad \text{(if normalized)}$$

- From Fourier sine series, we know that $\{ y_n(x) \}$ are a complete set on $[0, L] \Rightarrow$ any $f(x) = \sum_{n=1}^{\infty} a_n y_n(x)$ with $f(x)$ satisfying boundary conditions.
Another set of applications come from Laplace's equation $\nabla^2 \phi = 0$ (or generalizations).

We particularly consider how it plays out with different coordinate systems. Just as a warm-up, consider cylindrical coordinates.

Jackson covers telling us that in cylindrical coordinates

$$ \sqrt{\gamma^2} = \frac{1}{r} \partial_r (r \partial_r) + \frac{1}{\rho} \partial_\rho + \frac{\partial^2}{\partial z^2} $$

Look for separation of variables solution to $\nabla^2 \phi$: $\phi = R(r) \theta(\rho) Z(z)$

$$ \Rightarrow \frac{1}{r} \frac{d}{dr} (r \frac{dR}{dr}) R + \frac{1}{\rho} \partial_\rho \frac{d\theta}{d\rho} + R \frac{d^2}{dz^2} = 0 $$

Collect all $R$, $\theta$, $Z$ in separate terms by dividing by $R \theta \phi$:

$$ \frac{1}{r} \frac{d}{dr} (r \frac{dR}{dr}) + \frac{1}{\rho} \frac{d\theta}{d\rho} + \frac{1}{Z} \frac{d^2 Z}{dz^2} = 0 $$

no $\theta$'s

only $Z$'s

$$ \Rightarrow \frac{1}{Z} \frac{d^2 Z}{dz^2} = \text{constant} = k^2 $$

so $Z(z) \propto e^{\pm ikz}$

Now isolate $\phi$ term by multiplying by $\rho^2$

$$ \Rightarrow \frac{1}{\rho} \frac{d}{d\rho} (\rho \frac{dR}{d\rho}) + \frac{1}{\rho} \frac{d\theta}{d\rho} + k^2 \phi = 0 $$

only $\rho$'s

$$ \Rightarrow \frac{1}{R} \frac{d^2 R}{d\rho^2} = -m^2 $$

Bessel's equation!

Generalize $f(\rho)$ eigenvalue $w(\rho)$ "weight"

$$ \Rightarrow \text{Sturm-Liouville in general form} $$

(check similar exercise with $y^2$ in spherical, eg. $\frac{1}{r^2 \sin \theta} (\partial \frac{\partial f}{\partial \theta}) +$...
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General Sturm-Liouville form for \( y(x) \) equation:

\[
\frac{d}{dx} \left( f(x) \frac{dy}{dx} \right) - g(x) y + \lambda w(x) y = 0
\]

where \( w(x) > 0 \) on \( a \leq x \leq b \) \((x \in [a, b])\)

and boundary conditions:

\[
\begin{align*}
\alpha_1 y(a) + \beta_1 \frac{dy}{dx} \bigg|_{x=a} &= 0 \\
\alpha_2 y(b) + \beta_2 \frac{dy}{dx} \bigg|_{x=b} &= 0
\end{align*}
\]

Vocabulary:
- \( \alpha = 0 \Rightarrow \frac{dy}{dx} = 0 \) (Dirichlet conditions)
- \( \beta = 0 \Rightarrow y = 0 \) (Neumann conditions)

\( B.C.'s \):

Problem: Find \( \lambda \)'s for which there are non-trivial (i.e., \( y(x) \) is not identically zero) solutions. \( \Rightarrow \) eigenvalues and eigenfunctions, \( \lambda_n, y_n(x) \)

General solution: linear combination of orthogonal eigenfunctions

1. Orthogonal is with respect to weight \( w(x) \):

\[
\int_a^b y_m(x) y_n(x) w(x) \, dx = 0 \quad \text{if normalized, } \lambda_n \neq \lambda_m, \text{in general!}
\]

2. Completeness on \( x \in [a, b] \):

\[
f(x) = \sum_{n=0}^{\infty} a_n y_n(x) \quad \Rightarrow \quad a_n = \frac{\int_a^b f(x) y_n(x) w(x) \, dx}{\int_a^b (y_n(x))^2 w(x) \, dx} = \begin{cases} 1 & \text{if normalized} \\ \frac{1}{\infty} \int_a^b |y_n(x)|^2 \, dx & \text{if complex} \end{cases}
\]

\( \sum_{n=0}^{\infty} y_n(x) y_n(x) w(x) = S(x-x') \quad \int_1 \infty \frac{\sum_{n=0}^{\infty} y_n(x) y_n(x) w(x)}{\infty} \Rightarrow 1 = \sum_{n=0}^{\infty} |y_n(x)|^2 \quad x' = x_1 \wedge y_n < y_n \)

3. Eigenvalues \( \lambda_n \) are real

4. Self-adjoint: if \( Ly \equiv \frac{d}{dx} \left( f(x) \frac{dy}{dx} \right) - g(x) y \)

\[
\Rightarrow \int_a^b y_n(x) \frac{d}{dx} y_m(x) w(x) \, dx = \int_a^b y_m(x) \frac{d}{dx} y_n(x) w(x) \, dx \quad \text{because surface terms vanish from B.C.'s}
\]
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Proof of orthogonality: cf. \( \langle \psi_n | H | \psi_m \rangle \Rightarrow (E_n - E_m) \langle \psi_n | \psi_m \rangle = 0 \)
\( \Rightarrow \) non-degenerate \( \Rightarrow \langle \psi_n | \psi_m \rangle = \delta_{nm} \)

\[ y_n \times \left[ \frac{d}{dx} \left( f_n \frac{dy_n}{dx} \right) - g_n y_n + \lambda_n y_n \right] y_m = 0 \]

\[ y_m \times \left[ \frac{d}{dx} \left( f_m \frac{dy_m}{dx} \right) - g_m y_m + \lambda_m y_m \right] y_n = 0 \]

Subtract and integrate \( \int_b^a \) \( \frac{dy}{dx} [y_n \frac{d}{dx} (f_n \frac{dy_n}{dx}) - y_m \frac{d}{dx} (f_m \frac{dy_m}{dx})] = (\lambda_n - \lambda_m) \int_a^b y_n y_m \, dx \)

\[ \frac{dy}{dx} \left[ y_n \frac{d}{dx} (f_n \frac{dy_n}{dx}) - y_m \frac{d}{dx} (f_m \frac{dy_m}{dx}) \right] \bigg|_0^b \]

Like with Hamiltonian: partially integrate both terms:
\[ -\frac{dy}{dx} f_n \frac{dy_n}{dx} - (\lambda_n - \lambda_m) \frac{dy_n}{dx} f_m \frac{dy_m}{dx} = 0 \]

Surface terms?
\[ \frac{dy}{dx} [y_n f_n \frac{dy_n}{dx} - y_m f_m \frac{dy_m}{dx}] \bigg|_0^b \]

vanish if:
\( a) \) \( f(b) = f(0) = 0 \)
\( b) \) \( \alpha_n y + \beta_n \frac{dy}{dx} = 0 \) at each end
IF either \( y = 0 \) or \( \frac{dy}{dx} = 0 \), then done.
Otherwise \( \frac{dy}{dx} = \frac{\beta_n}{\alpha_n} \), \( y \Rightarrow \frac{\beta_n}{\alpha_n} \int_0^b y_n y_m \, dy \bigg|_0^a = 0 \)

Degeneracies? \( \lambda_n = \lambda_m \) for \( y_n \neq y_m \). Come back to this!
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If we consider $\nabla^2 \Phi = 0$ in spherical coordinates, separating the $\theta$ dependence from $\rho$ and $\Phi$ leads to

$$
\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{m^2}{\sin^2 \theta} + k = 0 \quad \text{for}\ P(\theta)
$$

Hence $x = \cos \theta$, $dx = -\sin \theta \, d\theta$ gives us

$$
\frac{d}{dx} \left( (1-x^2) \frac{dp}{dx} \right) - \frac{m}{1-x^2} + kP(x) = 0
$$

associated Legendre Functions

Check against general form $\Rightarrow \begin{cases} f(x) = -x^2 \\ g(x) = 0 \\ w(x) = 1 \end{cases}$

Where do Legendre polynomials come from?

If no dependence on $y$, $m = 0$ and look for power series solution:

Frobenius $y = \sum_{n=0}^\infty a_n x^n$

would produce $\Rightarrow a_{p+2} = \frac{p(p+1)}{(p+2)(p+1)} a_p \Rightarrow$ terminates for $k = l(l+1)$ for integer $l$.

If not terminated, $y_0$ converges for $-1 < x < 1$, but diverges for $x = \pm 1$, where we want a solution (e.g. for $\Phi$) $\Rightarrow$ require $k = l(l+1)$

$\Rightarrow \frac{d}{dx} \left( (1-x^2) \frac{dp_l}{dx} \right) + l(l+1)P_l = 0$ and choose $P_{l+1}(1) = 1$ for all $l$.

$\Rightarrow \int_{-1}^1 P_l(x) P_m(x) \, dx = \delta_{lm} \frac{\pi}{2l+1}$

See Legendre polynomial $L_n$, no for examples.

The $P_l$ satisfy various recursion relations.
If \( SL \) of form \( p(x) y'' + q(x) y' + r(x)y = 0 \)

Put \( g(x,t) = \frac{1}{(x-t)^2} \sum_{n=0}^{\infty} \frac{P_n(x)}{(2n)!} t^n \) \( \frac{d}{dx} \) for orthogonal polynomials

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Where do recursion relations come from?

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One source is a generating function that can be associated with a set of polynomials. This is a function whose expansion has the desired polynomials as coefficients.

For Legendre polynomials

\[ g(t,x) = \frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x) t^n \]

(This is Arken's notation, in Lea \( g(t,x) = G(x,t) \)).

Relates to solution to Laplace's equation \( \nabla^2 \phi = 0 \)

\[ \phi = \frac{q}{4\pi \rho_0 c_d} = \frac{q}{4\pi \rho_0 (r^2 + 2ar \cos \phi - d^2)} \]

\[ = \frac{q}{4\pi \rho_0 (r^2 + 2ar \cos \phi - d^2)} = \frac{q}{4\pi \rho_0} \left( \sum_{n=0}^{\infty} P_n(\cos \phi) \frac{1}{r^n} \right) \]

More on this later.

For now, note that \( g(t,1) = \frac{1}{1-t} = \sum_{n=0}^{\infty} t^n \Rightarrow P_n(1) = 1 \) matching coefficient.

Similarly, \( g(t,-1) = \frac{1}{t+1} \Rightarrow P_n(-1) = (-1)^n \).

Others: \( P_n(-x) = (-1)^n P_n(x) \) (parity) and \( P_n(\cos \phi) \leq P_n(1) = 1 \)

Now, \( \frac{d g(t,x)}{dt} = \frac{x-t}{1-2xt+t^2} \sum_{n=0}^{\infty} \frac{P_n(x)}{(2n)!} t^n = \sum_{n=0}^{\infty} \frac{P_n(x)}{(2n)!} t^n \\
\Rightarrow (1-2xt+t^2) \sum_{n=0}^{\infty} \frac{n!}{(2n)!} P_n(x) t^n + (t-x) \sum_{n=0}^{\infty} \frac{P_n(x)}{(2n)!} t^n = 0 \Rightarrow \text{equate coefficients of } t^n \\
\Rightarrow \text{differentiate wrt } x \text{ to get others. Look! Factor up as needed.} \)
Example of using recursion relations:  Lea problem 8.5.

Show using recursion relations (and integration by parts) that

$$\int_{-1}^{1} P_{l_1}(x) P_{l_2}(x) (1-x^2) \, dx = 0 \text{ if } l_1 \neq l_2$$

Assume we know

$$\int_{-1}^{1} P_{l_1}(x) P_{l_2}(x) \, dx = \frac{\delta_{l_1 l_2}}{2l_1+1}$$

and various recursion relations:

1. $l P_{l-1}(x) = (2l+1) x P_{l}(x) + (l+1) P_{l+1}(x) = 0$
2. $P_{l-1}(x) = P_{l+1}(x) - 2x P_{l}(x) + P_{l-1}(x)$
3. $l P_{l}(x) = x P_{l}(x) - P_{l+1}(x)$
4. $P_{l+1}(x) = x P_{l}(x) + (1-x^2) P_{l-1}(x)$

How do we proceed? Only one of $P_{l-1}$ has a $(1-x^2)$ factor, so use that first:

$$\Rightarrow (1-x^2) P_{l-1}(x) = \frac{-l_2}{2} \left[ x P_{l-1}(x) - P_{l-2}(x) \right]$$

$$\Rightarrow \int_{-1}^{1} \frac{\delta_{l_1 l_2}}{2l_1+1} \left[ x P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

$$= \frac{-l_2}{2} \left[ x \frac{d}{dx} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \right]_{-1}^{1} + \frac{l_2}{2} \int_{-1}^{1} \frac{d}{dx} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

Instead integrate by parts:

$$= \frac{-l_2}{2} \left[ \frac{d}{dx} \left[ x P_{l-1}(x) - P_{l-2}(x) \right] \right]_{-1}^{1} + \frac{l_2}{2} \int_{-1}^{1} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

$$= \frac{-l_2}{2} \left[ \left. x P_{l-1}(x) - P_{l-2}(x) \right|_{-1}^{1} \right] + \frac{l_2}{2} \int_{-1}^{1} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

$$= \delta_{l_1 l_2} \frac{d}{dx} \left[ \left. x P_{l-1}(x) - P_{l-2}(x) \right|_{-1}^{1} \right] + \frac{l_2}{2} \int_{-1}^{1} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

$$= \left. \frac{d}{dx} \left[ x P_{l-1}(x) - P_{l-2}(x) \right] \right|_{-1}^{1} + \frac{l_2}{2} \int_{-1}^{1} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

$$= l_2 \left[ \int_{-1}^{1} P_{l-1}(x) \, dx - \int_{-1}^{1} P_{l-2}(x) \, dx \right] + \frac{l_2}{2} \int_{-1}^{1} \left[ P_{l-1}(x) - P_{l-2}(x) \right] \, dx$$

$$= \frac{2l_2 \delta_{l_1 l_2}}{2l_1+1} \int_{-1}^{1} P_{l-1}(x) \, dx \quad \Box$$
alternative direct method in Arken,
but this is more instructive.

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What if an equation is not in the form of the S-L equation?

Example: Laguerre \( xy'' + (1-x)y' + ny = 0 \) on \( x \in [0, \infty) \)

The differential operator \( x \frac{d^2}{dx^2} + (1-x) \frac{d}{dx} \) is not self-adjoint.

Assume surface forms:

\[
\int y_1(x) \frac{d^2}{dx^2} y_2 \, dx = -\int (y_1' + y_1) \frac{d}{dx} y_2 \, dx + \int (y_1'' + 2y_1') y_2 \, dx
\]

\[
\int y_2 \frac{d}{dx} y_1 \, dx = -\int (y_2' + y_2) \frac{d}{dx} y_1 \, dx + \int (y_2'' + 2y_2') y_1 \, dx
\]

\[
\Rightarrow \int y_1 \frac{d^2}{dx^2} + (1-x) \frac{d}{dx} y_2 \, dx = \int \left[ x \frac{d^2}{dx^2} + (1-x) \frac{d}{dx} \right] y_1 y_2 \, dx
\]

not equal

What can we do? The solutions are unchanged if we multiply
by a positive function \( p(x) \) (That is, \( p(x) > 0 \) for all \( x \)).

Equate \( \frac{d}{dx} p(x) \frac{dy}{dx} + \lambda w y = f y'' + \frac{dx}{dx} y' - g y + \lambda w y \)

\[
=p x \left[ x y'' + (1-x) y' \right] + p(x) y
\]

\[
\Rightarrow \quad \text{max} = (p(x))^1/2, \quad \lambda = x \quad f(x) = x p(x), \quad \frac{df}{dx} = (1-x)p(x)
\]

\[
g(x) = 0 \quad \Rightarrow \quad \frac{df}{dx} = p + x p' = (1-x) p \quad \text{or} \quad p' = -p
\]

Solving, \( p(x) = e^x \) (The overall magnitude doesn't matter)

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

Laguerre polynomials! See laguerre_polynomials_1.nb for tests.

Laguerre polynomials show up in solutions to hydrogen atom in
3D quantum mechanics (cf. Hermite polynomials in solutions
to 1D harmonic oscillator)
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Consider solving a Laplace equation problem with spherical symmetry. Let example 8.2: Hollow sphere conductor except for insulating strip along equator ($\phi = \frac{\pi}{8}$). Radius is $a$.

Bottom half is grounded ($V=0$) while top half is held at $V=V_0$.

What is the potential inside the sphere?

Plan: No charges inside, so solve $\nabla^2 \Phi = 0$ subject to the boundary conditions $\Phi = V_0$ on the upper hemisphere and $\Phi = 0$ on the lower hemisphere.

Separate variables in spherical coordinates: $\Phi = R(\rho)\Theta(\theta)\phi(\phi)$

$$\nabla^2 \Phi = \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^2 \frac{\partial \Phi}{\partial \rho} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0$$

Usual game of substituting and dividing by $\Phi$ yields

$$\frac{1}{R} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) + \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\sin^2 \theta} \frac{d^2 \phi}{d\phi^2} = 0$$

Isolate simplest term: $R \Rightarrow$ multiply by $\rho^2 \sin^2 \theta$

$$\frac{\sin^2 \theta}{\rho} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) + \sin^2 \theta \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \frac{2 \cot \theta}{\sin^2 \theta} \frac{d^2 \phi}{d\phi^2} = 0$$

Only $\rho$ only $\theta$

$R$ need to be periodic in $\Theta$ with period $2\pi \Rightarrow \frac{1}{\rho^2 \sin^2 \theta} \frac{d^2 \phi}{d\phi^2} = -m^2 \Rightarrow E^2 \csc \phi$ (or $\sin \phi$), $m \in \mathbb{Z}$

Then isolate first term by dividing by $\sin^2 \theta$, to get

$$\frac{1}{R} \frac{d}{d\rho} \left( \rho^2 \frac{dR}{d\rho} \right) + \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \frac{m^2}{\sin^2 \theta} = 0$$

$$\Rightarrow \quad \epsilon = \text{only } \rho \quad \text{only } \theta$$

The $\Theta$ equation gives us again the associated Legendre equation we've already considered:

$$x = \cos \theta \Rightarrow \frac{d}{dx} \left( (1-x^2) \frac{d \Theta}{dx} \right) - \frac{m^2}{1-x^2} \Theta + k \Theta = 0.$$
What about the \( R(r) \) dependence when \( m = 0 \) (independent of \( \phi \)) and \( k = \lambda (\lambda + 1) \)?

\[
\frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) R = \lambda (\lambda + 1) R.
\]

If we let \( R(r) = \frac{u(r)}{r} \),

\[
\frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) u = \lambda u - \frac{\lambda (\lambda + 1)}{r^2} u = 0
\]

(\( \lambda \) is a constant; \( u \) is the angular part of the solution.)

Solutions are power laws \( u = r^p \)

\[
p(p-1)r^{p-2} - \lambda (\lambda + 1)r^{p-2} = 0 \Rightarrow p(p-1) = \lambda (\lambda + 1)
\]

\( R(r) = r^p \) \( \Rightarrow \) \( p \neq \lambda \)

So \( p = \lambda \), \( \lambda = \frac{1}{\lambda + 1} \)

This means that the general eigenfunction expansion for anisotropy with \( \phi \) dependence

\[
\Phi(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_l^m e^{im\phi} P_l^{(\lambda)}(\cos \theta)
\]

and \( A_l^m, B_l^m \) are fixed by the boundary conditions in \( \theta \).

So back to our 2-hemisphere problem,

i) There's nothing at \( r = 0 \), so \( \Phi \) can't diverge. \( \Phi \) \( \Rightarrow \) \( A_0^0 = 0 \) \( \forall \lambda \).

ii) Evaluate \( \Phi(\phi) \) at \( r = a \)

\[
\sum_{l=0}^{\infty} A_l^0 \alpha^l P_l^0(x) = \begin{cases} 
1 & \text{if } x > 0 \\
0 & \text{if } x < 0
\end{cases}
\]

(\( \alpha^l \) for \( \frac{\pi}{2} < \theta < \pi \))

Use orthogonality to project out the \( A_l^0 \) s.

\[
\sum_{l=0}^{\infty} A_l^0 \int_0^1 P_l^0(x)^2 dx = \int_0^1 P_l^0(x) dx \Rightarrow \sum_{l=0}^{\infty} \frac{2}{2l+1} S_l \text{ on left side}
\]

exchange \( l, x \) \( \Rightarrow \) \( A_l^0 = \frac{2}{2l+1} V \int_0^1 P_l^0(x) dx \)
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How do we evaluate \( \int_0^1 p_l(x) \, dx \)?

For \( l=0 \), \( \int_0^1 1 \, dx = 1 \).

For \( l \geq 0 \), we can use the recursion relation
\[
p_l(x) = \frac{1}{2l+1} \left( p_{l+1}(x) - p_{l-1}(x) \right)
\]
or the Rodrigues formula:
\[
p_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2-1)^l
\]

or simply ask Mathematica:

\[
\int_0^1 p_l(x) \, dx = \text{Integrate} \left[ \text{LegendreP}[l,x], \{x,0,1\} \right]
\]

\[
= \frac{\sqrt{\pi}}{2^l l!} \frac{1}{\Gamma(1+\frac{l}{2}) \Gamma(3+\frac{l}{2})}
\]

Which is 0 for even \( l > 0 \).

This is clear on \( \int_0^1 p_l(x) p_m(x) \, dx \) for even \( l \), so \( \delta_{l0} \).

\[
\Rightarrow \phi(l, \theta) = \frac{\sqrt{\pi}}{2^l l!} \frac{1}{\Gamma(1+\frac{l}{2}) \Gamma(3+\frac{l}{2})} \left( \frac{1}{2} \right)^l P_l(\cos \theta)
\]

See LegendrePolynomial in.nb

"How would we solve this numerically?"

"Is there a clear preference with the analytic solution given above?"
As an example of how the expansion works when we don't have azimuthal symmetry ($\phi$ independent), let's consider the same split conducting sphere, but now turned on its side:

This example is considered in detail in Lau Example 3.3, including showing that it reproduces the same answer from before when the coordinates are transformed appropriately. We will focus on the setup. Here is now a $\phi$ dependence, so we will start with the general expansion for a solution to $\nabla^2 \Phi = 0$:

$$\Phi(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left( A_{l} \alpha_l + \beta_{l} \beta_l \right) r^{-l+1} Y_{lm}(\theta, \phi)$$

Goal: use the boundary condition to find the $A_l$'s.

Gain: $\Phi(r=a, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{l} \alpha_{l} \left| Y_{lm}(\theta, \phi) \right| = \begin{cases} V_0 & \text{if } 0 \leq \theta < \pi/2 \\ 0 & \text{if } \pi/2 \leq \theta < \pi \end{cases}$

Plan: Project out $A_l$ using the orthogonality of $\Re Y_{lm}$:

$$\Rightarrow \int \delta \phi \Phi(r=a, \theta, \phi) d\phi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{l} \alpha_{l} \int \delta \phi \left| Y_{lm}(\theta, \phi) \right| Y_{lm}(\theta, \phi)$$

What would we get if the $\phi$ integral was $0$ to $2\pi$?

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{l} \alpha_{l} \int_{0}^{2\pi} \sin \theta \, d\theta \int_{0}^{2\pi} \, d\phi V_0 Y_{lm}^{*}(\theta, \phi) \int_{0}^{\pi} \, d\phi$$

so we're basically done. Let's expose $\Re \phi \gamma$ dependence:

$$A_{l} = \frac{V_0}{\alpha_{l} \sqrt{4\pi \left( l(l+1) \right)}} \int_{0}^{\pi} P_{l}^{m}(x) dx \int_{0}^{\pi} e^{im\phi} \frac{d\phi}{lhm}$$

For $m > 0$:

$$\left( 1 - \frac{m(m+1)}{l^2} \right) = 0 \text{ unless m is odd}$$
Let's look at $A_{lm}$ for $m = 0$, which we need to treat separately.

For $l = 0, m = 0$, $Y^{m}_{l=0} = \frac{1}{\sqrt{4\pi}}$.

\[ A_{00} = V_0 \int \frac{1}{\sqrt{4\pi}} \, d\phi = \frac{V_0}{\sqrt{4\pi}} \]

**(Type error, see errata)**

Suppose $m = 0$ but $l \neq 0$. Recall $P^m_{l-1}(x) = P^m_l(x)$: Legendre polynomial.

\[ \Rightarrow \int P^m_l(x) \, dx = \int P^m_{l-1}(x) \, dx = \int P^m_l(x) P^m_{l-1}(x) \, dx = 2 \delta_{l0} \]

So only $l = 0$ when $m = 0$.

When $m = 0$, $\int \frac{(1 - (x^2))^{m/2}}{\sqrt{2\pi}} \, dx = 0$ unless $m$ is odd. But if $m$ is odd and $l$ even, then $P^m_l(x)$ is odd, so integrates to zero.

Besides the $l = 0, m = 0$ term, the expansion is over $l$ odd, $m$ odd.

We are left with the integral $I_{lm}$:

\[ I_{lm} = \frac{1}{(2\pi)^{1/2}} \int_{-1}^{1} P^m_l(x) \, dx = \frac{\pi}{2} P^m_l(0) P^m_{l-1}(0) \frac{(l+m)!}{(l+1)!} \frac{1}{(l-m)!} \]

\[ \int_{-1}^{1} P^m_l(x) \, dx = \begin{cases} 0, & m \text{ odd;} \\ \frac{2\pi}{2l+1}, & m \text{ even.} \end{cases} \]

\[ \Rightarrow \frac{1}{(2\pi)^{1/2}} \int_{-1}^{1} P^m_l(x) \, dx = \begin{cases} \frac{2\pi}{2l+1}, & m \text{ even;} \\ 0, & m \text{ odd.} \end{cases} \]

\[ = \frac{2\pi}{2l+1} \frac{1}{(2\pi)^{1/2}} \int_{-1}^{1} P^m_l(x) \, dx \]

\[ = \frac{2\pi}{2l+1} \frac{1}{(2\pi)^{1/2}} \int_{-1}^{1} P^m_l(x) \, dx \]

\[ \Rightarrow \Phi(r, \theta, \phi) = V_0 \left[ \frac{1}{a} + \sum_{l=0}^{\infty} \sum_{m= \pm l}^{l} \frac{\delta_l(2l+1)(l+m)!}{l!} P^m_l(0) P^{m}_{l-1}(0) \frac{2\pi}{2l+1} \right] \]

\[ \frac{2\pi}{2l+1} \frac{1}{(2\pi)^{1/2}} \int_{-1}^{1} P^m_l(x) \, dx \]

\[ \Rightarrow \Phi(r, \theta, \phi) = V_0 \left[ \frac{1}{a} + \sum_{l=0}^{\infty} \sum_{m= \pm l}^{l} \frac{\delta_l(2l+1)(l+m)!}{l!} P^m_l(0) P^{m}_{l-1}(0) \frac{2\pi}{2l+1} \right] \]

\[ \frac{2\pi}{2l+1} \frac{1}{(2\pi)^{1/2}} \int_{-1}^{1} P^m_l(x) \, dx \]

Not immediately obvious, but this is real, need $m, \pm l, m$ to be the same.

First terms: $V_0 = \left[ \frac{1}{5} + \frac{3}{128} \phi \sum \sin \sin \phi + \frac{7}{128} \phi \sin \phi \right] \left[ \sum \sin \sin \phi \right]$.
\[ \Phi(r, \theta, \phi) = \frac{V_0}{2} \left( 1 - \sum_{l=1}^{\infty} \frac{(2l+1)}{l} \frac{\rho^l}{\rho} \rho_l(\cos \theta) \right) \]

should be the same potential \( \Rightarrow \text{shown in leu.} \)

What if the equation is not Laplace's equation.
E.g., the wave equation in spherical coordinates:
\[ \nabla^2 F = \frac{1}{c^2} \frac{\partial^2 F}{\partial t^2} = 0 \]

First transform in time \( \Rightarrow k^2 = \frac{\omega^2}{c^2} \)
\[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial F}{\partial r} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial F}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 F}{\partial \phi^2} + k^2 F = 0 \]

What if a time-independent Schrödinger equation with \( V(\mathbf{r}) \)?
Same except \( k^2 F \rightarrow V(\mathbf{r}) F - EF \) [wrote \( E \rightarrow \Phi(r, \theta, \phi) \) energy]

Separate yet again as \( F = R(r) \Theta(\theta) \Phi(\phi) \)
\( \Rightarrow \Theta \) and \( \Phi \) equations will be the same as for \( \nabla^2 \phi = 0 \)
so very general.

But \( r \) equation will depend on wave equation vs. \( S \)-eqn vs. ...

wave equation:
\[ \frac{1}{R} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + k^2 R^2 - \ell(\ell+1) = 0. \]

This can be converted to Bessel's equation and we read off that
this combination called
\[ R(\mathbf{r}) = J_{\frac{1}{2}}(kr) \]
\( \Rightarrow \) "spherical Bessel function": \( J_\ell(z) = \frac{1}{\sqrt{2\pi}} \frac{\sin z - \cos z}{z} \)
(and independent solution not regular at origin)
\( J_0(z) \sim z^0 \) for small \( z \), satisfies recursion relations. Try functions:
\[ J_0(z) = \frac{\sin z}{z}, \quad J_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}, \quad J_2(z) = \left( \frac{3}{2} - \frac{1}{2} \right) \sin z - \frac{3}{2} \cos z \]
You can use spherical harmonics to find an expansion for \(|\frac{1}{|\mathbf{r} - \mathbf{r}'|}|^2\):

\[
\frac{1}{|\mathbf{r} - \mathbf{r}'|^2} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{n^2}{r^2} Y_{lm}(\theta, \phi) Y_{lm}^*(\theta', \phi')
\]

This could be used for angles at \(\frac{\pi}{2}\) and angles at \(\frac{\pi}{4}\) depending on whether \(r<\frac{1}{r'+h}\)

Useful for EM problems: electrostatics, magnetostatics

Another very useful expansion is of a plane wave:

\[
\langle \psi | \Phi_n | \rangle = \frac{\exp(-iE_n t)}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} \frac{\sqrt{l(l+1)}}{2\pi} (i)Y_l^m(kr, \Omega) P_l(\cos \theta)
\]

where \(P_l(\cos \theta)\) is the Legendre polynomial.

Separate out the dependence \(m \rightarrow l \rightarrow \text{dependence}

\Rightarrow "partial wave expansion", eg. for central potential in quantum mechanics.

In Problem 4, solve 3D square well problem (Bonus)

cf. one d \(\dot{1} \quad \dot{2} \quad \dot{3} \quad \dot{4} \)

match sines and cosines in \(I\) to exponentials in \(II, III\), analogy in 3D

with \(l>0\) is matching regular and modified spherical Bessel functions.
Orthogonal Polynomials

- orthogonal on \([a, b]\) with weight function \(w(x)\)
- satisfy recursion relations
- have a generating functional and Rodrigues-type formula

Common examples

<table>
<thead>
<tr>
<th></th>
<th>(a)</th>
<th>(b)</th>
<th>(w(x))</th>
<th>normalization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Legendre</td>
<td>(-1)</td>
<td>1</td>
<td>1</td>
<td>(\int_1^1 [P_n(x)]^2 dx = \frac{2}{2n+1})</td>
</tr>
<tr>
<td>Hermite</td>
<td>(-\infty)</td>
<td>(\infty)</td>
<td>(e^x)</td>
<td>(\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} dx = \frac{n!}{\sqrt{\pi}})</td>
</tr>
<tr>
<td>Laguerre</td>
<td>0</td>
<td>(\infty)</td>
<td>(x^e^{-x})</td>
<td>(\int_0^{\infty} [L_n(x)]^2 e^{-x} dx = \frac{n!}{n^{n/2}})</td>
</tr>
<tr>
<td>Chebyshev</td>
<td>(-1)</td>
<td>1</td>
<td>(\frac{1}{\sqrt{1-x^2}})</td>
<td>(\int_{-1}^{1} [C_n(x)]^2 \left(\frac{1-x^2}{(1-x^2)^{1/2}}\right) dx = \frac{n!}{n^{n/2}})</td>
</tr>
</tbody>
</table>

Other spellings are common!

Call them generically \(p_n(x)\) with weight \(w(x)\) on \([a, b]\).

We've encountered them as solutions to differential equations, but an alternative construction, up to normalization, is to require

\[
\int_a^b w(x) x^k p_n(x) \, dx = 0 \quad \text{for all } 0 \leq k < n \quad \text{with } p_0(x) = 1.
\]

So \(p_1(x)\) from \(\int_a^b w(x) x \, p_0(x) \, dx = 0\), \(p_2(x)\) from \(\int_a^b w(x) x^2 \, p_1(x) \, dx = 0\) \(\Rightarrow c \Rightarrow p_2(x)\) and so on. For \(w(x) = 1\), \(a = -1\), \(b = 1\), generates Legendre polynomials with leading coefficient \(1\): \(p_0(x) = 1, p_1(x) = x, p_2(x) = x^2 - \frac{1}{3}, \ldots\)
How can we use these to do approximate calculations of
integrals? (called numerical quadrature).

We can transform \( \int f(x) \, dx \) possibly after breaking it
into pieces, into an integral from \(-1\) to \(1\).

\[ I = \int_{-1}^{1} f(x) \, dx \]

We seek a quadrature rule with \( N \) points:

\[ I = \sum_{i=1}^{N} w_i f(x_i) \]

where \( x_i, w_i \) are fixed (ie don't change for different \( f(x) \)).

Suppose \( N=3 \) and we require \( x = -1, x = 0, x = 1 \)
On small interval, smooth functions looks like (low-order)
polynomials (Taylor expansion) \( \Rightarrow \) approximate as quadratic.

\[ f(x) = ax^2 + bx + c \]
is perfectly integrated for any \( a, b, c \)

\[ \frac{1}{2} \int_{-1}^{1} (ax^2 + bx + c) \, dx = \frac{a}{3} + \frac{b}{2} + c \]

\[ \Rightarrow \sum_{i=1}^{3} w_i f(x_i) = w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3) \]

with \( x_1 = -1, x_2 = 0, x_3 = 1 \) \( \Rightarrow f(1) = a + b + c \)
\[ f(0) = c \]
\[ f(-1) = a - b + c \]

\( \Rightarrow (a - b + c) w_1 + c w_2 + (a + b + c) w_3 = 2a/3 + 2c \)

\( \Rightarrow \frac{3}{2} w_1 + w_2 + w_3 = 2a/3 + 2c \)

\[ w_1 = \frac{4}{3}, \quad w_2 = w_3 = \frac{1}{3} \]

Simpson's rule.

\( \Rightarrow w_2 = w_3 = \frac{1}{3} \)
Simpson's rule is exact for polynomials of degree 2.
In general, a Taylor series with \( N \) equally spaced points yields a rule that integrates a polynomial of degree \( N-1 \) or \( N \), depending on whether \( N \) is odd or even.

Stitch Simpson's together:
\[
\frac{1}{3}f(x_1) + \frac{4}{3}f(x_2) + \frac{2}{3}f(x_3) + \frac{4}{3}f(x_4) + \frac{1}{3}f(x_N)
\]

- How can we do better with an \( N \)-point rule?
  - let the \( x_i \) vary rather than being equally spaced
  - integrate \( N-1 \) polynomial exactly
  - Gaussian quadrature

- Basic idea: given \( w(x) \) and \( N \), construct the orthogonal polynomials \( p_0(x), ..., p_{N-1}(x) \).

- Now consider all \( h(x) \) polynomials of degree \( 2N-1 \) or less
  - Divide \( h(x) \) by \( p_{N-1}(x) \)
    - \( q(x) \) and remainder \( r(x) \)
  - both of degree less than \( N \) so both orthogonal to \( p_N(x) \)

\[
\begin{align*}
  I_N &= \int_a^b w(x)h(x) \, dx \\
  &= \int_a^b w(x)q(x)p_N(x) \, dx + \int_a^b w(x)r(x) \, dx
\end{align*}
\]

Integration rule
\[
\begin{align*}
  I_N &= \sum_{i=1}^{N} w_i h(x_i) \\
  &= \sum_{i=1}^{N} w_i q(x_i)p_N(x_i) + \sum_{i=1}^{N} w_i r(x_i)
\end{align*}
\]

- want to duplicate
  - vanishing of flat integral and get something exactly
  - choose the \( x_i \) at \( N \) zeros

- use freedom of \( N \) \( w_i \)'s so of \( r(x) \)

\( \text{This term is zero!} \)

\( \text{This term integrated exactly!} \)

\[
\begin{bmatrix}
p_0(x_1) & \cdots & p_0(x_N) \\
p_1(x_1) & \cdots & p_1(x_N) \\
p_2(x_1) & \cdots & p_2(x_N) \\
\vdots & \ddots & \vdots \\
p_{N-1}(x_1) & \cdots & p_{N-1}(x_N)
\end{bmatrix}
\begin{bmatrix}
w_1 \\
w_2 \\
w_3 \\
\vdots \\
w_N
\end{bmatrix}
= \begin{bmatrix}
\int_a^b w(x)p_0(x) \, dx \\
\int_a^b w(x)p_1(x) \, dx \\
\int_a^b w(x)p_2(x) \, dx \\
\vdots \\
\int_a^b w(x)p_{N-1}(x) \, dx
\end{bmatrix}
\]

- solve for \( w_i \)'s!
Example problems:

Consider \( I = \int_0^3 (4t)^{1/2} \, dt = 4.6666 \)

We can always switch to \([-1,1]\) using

\[
\int_a^b f(x) \, dx = \frac{b-a}{2} \int_{-1}^1 f \left( \frac{b-a}{2} x + \frac{a+b}{2} \right) \, dx = \frac{b-a}{2} \sum_{i=1}^n \omega_i f \left( \frac{b-a}{2} x_i + \frac{a+b}{2} \right)
\]

Choose \( t = \frac{x}{2} + \frac{a+b}{2} \) 

So for \( I \), switch to \( x = -t + \frac{a+b}{2} \Rightarrow I = \frac{3}{2} \int_{-1}^1 \left( \frac{3}{2} x + \frac{a+b}{2} \right)^{1/2} \, dx \)

See gauss_quad_test.py for these tests.

\( N = 3 \) Simpson's rule yields \( I_{\text{simpson}} = 4.662228 = 10^{-3} \) relative error

\( N = 3 \) Gauss-Legendre nodes and weights are

\( x_1 = -x_3 = -0.774597, x_2 = 0, \ \omega_1 = \omega_3 = 0.555556, \ \omega_2 = 0.888888 \)

Yields \( I_{\text{Gauss-Legendre}} = 4.66683 \Rightarrow 0.3 \times 10^{-4} \) relative error

\( \Rightarrow \) \( \approx 30 \) times more accurate with same \# of evaluations!

Try on \( N = 3 \) Gauss-Laguerre integration with \( \int_0^\infty (x^3 + 3x + 5)e^{-x} \, dx = 10 \)

Perfect! Also for \( x^4 - 2x^3 + 14x^2 + 3x + 5 \).

Pretty good for \( \int_0^\infty \sin x \, e^{-x} \, dx \). Fails for \( x^6 - 2x^3 + 7x^2 + 3x + 8 \)

\( \text{order is greater} \)

Plan 3.3-1 = 5
Gaussian quadrature follow-up (2 examples)

\[ \int_{-1}^{1} f(x) \, dx = \sum_{i=1}^{N} w_i \cdot f(x_i) \]

where the \( x_i \)'s are the \( N \) roots (zeros) of \( P_N(x) \) [Legendre polynomial].

Features:
- Symmetric points about \( x = 0 \)
- As \( N \) increases, accumulation of points near \( -1 \) and \( 1 \), but never at \( -1, 1 \)
- For odd \( N \), no point at zero. If \( f(x_0) \) has a pole, then one gets \( P_{N/2}/f_0 \) (principle value)

\[ \int_{0}^{\infty} e^{-x} \, dx = \sum_{i=1}^{N} w_i \cdot f(x_i) \]

- Both are exact if \( f(x) \) is a polynomial of degree \( \leq N-1 \)
- There are standard algorithms to find the \( w_i \)'s, but usually you would use a packaged routine to calculate them.

- If you consider the \( x_i \)'s and \( w_i \)'s and \( f(x_i) \)'s as vectors, then \( I = \text{dot product of } \overrightarrow{W} \text{ and } \overrightarrow{F} \)
  - Mathematica:
    \[
    x_{\text{nodes}} = \{ \ldots, \ldots, \ldots \} \\
    x_{\text{weights}} = \{ \ldots, \ldots, \ldots \} \\
    \Rightarrow I \text{ from } f[x_{\text{nodes}}, x_{\text{weights}}]
    \]
- Look at `gauss_quad_test.m` for examples.