

Supplemental Notes on Mathematical Methods

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CHAPTER 1

Sturm-Liouville Differential Equation

1.1 Motivation

Many of the problems we have studied follow from general properties of the Sturm-Liouville (SL) problem. In these problems, a system is governed by the differential equation of the form

$$\frac{d}{dx} \left[p(x) \frac{d}{dx} \right] \phi(x) + q(x)\phi(x) = -\lambda r(x)\phi(x) \quad (1.1)$$

for $x \in [a, b]$, where $a, b \in \mathbb{R}$ and some real functions p, q, r , where $p(x), r(x) > 0$ for $x \in (a, b)$ ¹. This is in essence an eigenvalue problem, where we would like to determine the eigenvalues λ and corresponding eigenfunctions $\phi(x)$ which satisfy Eq. (1.1) for a given set of p, q, r .

For example, the Schrödinger equation, Bessel's equation, and Legendre's equation all fall under this category. Clearly, the particular properties that determines a system's unique behavior depend on p, q, r , but the general methods by which we uncover these all follow the same generic trend which follow from general behaviors of systems with a Sturm-Liouville description.

1.2 Boundary Conditions

Since the Eq. (1.1) is a second-order differential equation, we have two linearly independent solutions $y_{1,2}$ for a given set of functions p, q, r , and a general solution $y = \alpha_1 y_1 + \alpha_2 y_2$, where $\alpha_{1,2}$ are constants. These constants are determined by boundary conditions at $x = a, b$ by specifying (1) $y(a)$ and $y(b)$ [Dirichlet BCs], (2) $y'(a)$ and $y'(b)$ [Neumann BCs], or (3) $c_a y(a) + d_a y'(a)$ and $c_b y(b) + d_b y'(b)$ [Robin BCs]. For the most part, we focus on Dirichlet BCs

¹Note that the endpoints are excluded here!

(e.g. specifying the value of the wave function) and Neumann (e.g. specifying the surface charge density). It is rare in the textbook problems that a linear combination of the function and its derivative are specified since these linear combinations are not usually related to a physical quantity. For the development of general properties, though, we will reference these kind of BCs, but Dirichlet and Neumann BCs are recovered by setting $d_{a,b} = 0$ and $c_{a,b} = 0$, respectively.

Finally, in some cases, a fourth distinct set of BCs can be specified, which are called periodic BCs. As the name suggests we either have $y(a) = y(b)$ or $y'(a) = y'(b)$.

1.3 Definitions

Let us define a couple of terms that will be used to identify the type of equation we consider.

1. A *regular* SL system is one such that homogeneous mixed BCs are given: $c_a y(a) + d_a y'(a) = 0$ and $c_b y(b) + d_b y'(b) = 0$
2. A *periodic* SL system is one such that periodic BCs are specified and $p(a) = p(b)$
3. A *singular* SL system is one where any of the following occur:
 - $p(a) = 0$, no BC at a is given, and the BC at b is homogeneous mixed (Note: solutions must be bounded at $x = a$)²
 - $p(b) = 0$, no BC at b is given, and the BC at a is homogeneous mixed (Note: solutions must be bounded at $x = a$)
 - $p(a) = p(b) = 0$ and no BCs are given (solutions must be bounded at both $x = a, b$.)
 - $a \rightarrow -\infty$ and $b \rightarrow \infty$ such that the equation is defined on \mathbb{R} (Note: solutions must be square-integrable on \mathbb{R})³

1.4 Properties of the Sturm-Liouville System

1.4.1 Sturm-Liouville Operator

Let $\mathcal{L}^2([a, b], r(x), dx)$ be the Hilbert space of square integrable functions on the interval $[a, b]$ with inner product

$$(f, g) = \int_a^b r(x) f^*(x) g(x) dx. \quad (1.2)$$

It is for this reason that $r(x)$ is sometimes denoted a *weight* function.

²A function f is bounded at x if $|f(x)| < M$ for some M .

³A function f is square-integrable if $\int_{-\infty}^{\infty} |f(x)|^2 < \infty$ (i.e. the integral is convergent and bounded).

Denote the linear differential operator

$$\hat{L} = -\frac{1}{r(x)} \left[\frac{d}{dx} p(x) \frac{d}{dx} + q(x) \right], \quad (1.3)$$

and let $\mathcal{H} \subset \mathcal{L}^2$ be the subspace of functions which are square integrable and satisfy a given set of BCs. The SL problem can then be stated as

$$\hat{L}\phi(x) = \lambda\phi(x), \quad (1.4)$$

and because of this relation we call L the SL operator. Effectively, we have explicitly rewritten Eq. (1.1) as an eigenvalue equation. We now study generally some properties of the SL operator and its spectrum and space of eigenfunctions.

1.4.2 Facts about solutions and eigenvalues of the Sturm-Liouville problem

Theorem 1: *The SL operator is self-adjoint.* Recall that the adjoint A^\dagger of an operator A is defined by the equality $(A^\dagger f, g) = (f, Ag)$, and a self-adjoint operator is one such that $A^\dagger = A$. The proof is as follows for the SL operator. Consider the inner product

$$\begin{aligned} (f, Lg) &= \int_a^b r f^* \hat{L}g \, dx = \int_a^b f^* \left[-\frac{d}{dx} \left(p \frac{d}{dx} \right) + q \right] g \, dx \\ &= - \int_a^b f^* \frac{d}{dx} \left(p \frac{d}{dx} \right) g \, dx + \int_a^b [qf]^* g \, dx \\ &= - \left[f^* p g' \right]_a^b + \int_a^b p \frac{df^*}{dx} \frac{dg}{dx} \, dx + \int_a^b [qf]^* g \, dx \\ &= \left[p \left(\frac{df^*}{dx} g - f^* \frac{dg}{dx} \right) \right]_a^b + \int_a^b \left\{ \left[-\frac{d}{dx} p \frac{d}{dx} + q \right] f \right\}^* g \, dx \\ &= \int_a^b (\hat{L}f)^* g \, dx = (\hat{L}f, g). \end{aligned} \quad (1.5)$$

Note that the boundary term from the integrations by parts is zero for certain homogeneous BCs we discussed above. This is straightforward to see for homogeneous Dirichlet BCs ($f(a) = f(b) = g(a) = g(b) = 0$) and Neumann BCs ($f'(a) = f'(b) = g'(a) = g'(b) = 0$).

Theorem 2: *The eigenvalues of \hat{L} are real.* Suppose $\phi_\lambda \neq 0$ is the function with corresponding eigenvalue λ . That is $\hat{L}\phi_\lambda = \lambda\phi_\lambda$. Since \hat{L} is self-adjoint, we can write

$$\begin{aligned} (\hat{L}\phi_\lambda, \phi_\lambda) &= (\phi_\lambda, \hat{L}\phi_\lambda) \\ (\lambda\phi_\lambda, \phi_\lambda) &= (\phi_\lambda, \lambda\phi_\lambda) \\ \lambda^*(\phi_\lambda, \phi_\lambda) &= \lambda(\phi_\lambda, \phi_\lambda) \\ \lambda^* &= \lambda \end{aligned} \quad (1.6)$$

Theorem 3: If ϕ_λ and ϕ_μ correspond to distinct eigenvalues λ and μ , then ϕ_λ and ϕ_μ are orthogonal (i.e. $(\phi_\lambda, \phi_\mu) = 0$). The proof of this fact is straightforward. The eigenfunctions satisfy $\hat{L}\phi_\lambda = \lambda\phi_\lambda$ and $\hat{L}\phi_\mu = \mu\phi_\mu$. It follows then that

$$\begin{aligned} (\hat{L}\phi_\lambda, \phi_\mu) &= (\phi_\lambda, \hat{L}\phi_\mu) \\ \lambda(\phi_\lambda, \phi_\mu) &= \mu(\phi_\lambda, \phi_\mu). \end{aligned} \quad (1.7)$$

Rewriting we have

$$[\lambda - \mu](\phi_\lambda, \phi_\mu) = 0 \Rightarrow (\phi_\lambda, \phi_\mu) = 0 \quad (1.8)$$

since by assumption $\lambda \neq \mu$.

Theorem 4: The spectrum of \hat{L} is non-degenerate. That is to say that if ϕ_1 and ϕ_2 correspond to the same eigenvalue, then $\phi_2 = c\phi_1$, or ϕ_1 and ϕ_2 are linearly dependent. We prove this by contradiction. Suppose that there exists $\phi_1 \neq \phi_2$ such that $\hat{L}\phi_{1,2} = \lambda\phi_{1,2}$. We then have

$$\begin{aligned} \phi_2 \hat{L}\phi_1 - \phi_1 \hat{L}\phi_2 &= -\frac{1}{r(x)} \left[\phi_2 \frac{d}{dx} (p\phi_1) - \phi_1 \frac{d}{dx} (p\phi_2) \right] = 0 \\ &= -\frac{1}{r(x)} \frac{d}{dx} p(x) \underbrace{[\phi_1' \phi_2 - \phi_1 \phi_2']}_{W[\phi_1, \phi_2]} = 0. \end{aligned} \quad (1.9)$$

We then have

$$p(x)W[\phi_1(x), \phi_2(x)] = c. \quad (1.10)$$

Notice that for homogeneous BCs,

$$W[\phi_1(x), \phi_2(x)] = \frac{d\phi_1}{dx} \phi_2 - \phi_1 \frac{d\phi_2}{dx} = 0. \quad (1.11)$$

This is simple to see for pure Dirichlet and Neumann BCs since either the function or the derivative is zero at the boundaries. Thus, we have a separable 1st order equation with solution

$$\phi_1(x) = c\phi_2(x). \quad (1.12)$$

Theorem 5: The set of eigenfunctions is a basis for \mathcal{H} . Equivalently, the set of eigenfunctions $\{\phi_\lambda\}$. Let us assume for now that \hat{L} has a countable spectrum, allowing us to label the eigenfunctions by natural numbers such that eigenvalue λ_n corresponds to eigenfunction ϕ_n . A rigorous statement of completeness is this: if $\psi(x)$ is any function in \mathcal{H} ,

$$\lim_{n \rightarrow N} \|\psi(x) - \sum_{k=1}^n c_k \phi_k\|, \quad (1.13)$$

where N is the number of discrete eigenvalues in the spectrum of \hat{L} (possibly infinite). Note that the coefficients $c_k = (\phi_k, \psi)$ and the norm $\|\cdot\|$ is defined as $\|\psi\| = \sqrt{(\psi, \psi)}$. Another way of stating completeness is that

$$\sum_n \phi_n^*(x') \phi_n(x) = \delta(x - x'). \quad (1.14)$$

This is equivalent since any function $\psi \in \mathcal{H}$ can be expressed as

$$\psi(x) = \int_a^b dx' \psi(x') \delta(x - x') = \sum_n \phi_n(x) \underbrace{\int_a^b dx' \phi_n^*(x') \psi(x')}_{c_n}. \quad (1.15)$$

Note that there was no “proof” here. We really just posited that the eigenfunctions of \hat{L} forms a complete basis. The proof is quite involved and requires a more formal and advanced treatment than is within the scope of this discussion. We will assume that the mathematicians who have proven this result are quite competent⁴ and will simply take it as fact. It is essential that this theorem is true, though, since many of our problems hinge on the completeness of the eigenfunctions and our ability to expand a solution of an arbitrary SL problem in this basis.

⁴This argument is a bit flippant and depends on the assumption that the probability of a mistake being missed in the proof going to zero as the number of people who validated it goes to infinity (law of large numbers).

CHAPTER 2

Gamma Function

The Gamma function appears in many places, including our treatment of specific cases of the Sturm-Liouville problem and its solution. Before moving on then, we will take a look at the Gamma function and work out some of its useful properties in a more elaborate way than in our courses, which primarily highlighted its definition and properties without indicating how they arise.

2.1 Definition

The Gamma function is really an analytic continuation of the factorial function to the complex plane. Let us define

$$\Gamma(z) = \int_0^{\infty} x^{z-1} e^{-x} dx. \quad (2.1)$$

It is simple to derive its defining recursion property via integration by parts

$$\Gamma(z+1) = \int_0^{\infty} x^z e^{-x} dx = -x^z e^{-x} \Big|_0^{\infty} + z \int_0^{\infty} x^{z-1} e^{-x} dx = z\Gamma(z). \quad (2.2)$$

If $z \in \mathbb{N}^1$, then

$$\Gamma(n+1) = n\Gamma(n) = \dots = n(n-1)\dots(3)(2)(1)\Gamma(1) = n!. \quad (2.3)$$

Note that

$$\Gamma(1) = \int_0^{\infty} e^{-x} dx = -e^{-x} \Big|_0^{\infty} = 1. \quad (2.4)$$

One important observation is that the integral definition above only applies to $z \in \mathbb{C}^2$ such that $\operatorname{Re}\{z\} \geq 0$. If $\operatorname{Re}(z) < 0$, then the integrand is divergent as

¹If you are not familiar with this notation $\mathbb{N} = \{1, 2, 3, \dots\}$ is just the set of natural numbers.

²The set \mathbb{C} is just the set of complex numbers.

$x \rightarrow 0$. We can however, use analytic continuation again to define the Gamma function for z with negative real parts using Eq. (2.3):

$$\Gamma(z) = \frac{1}{z} \Gamma(z+1). \quad (2.5)$$

Essentially, one applies this recursion relation N times until $z + N \geq 0$.

2.2 Important Identities

A common value that is needed is $\Gamma(1/2)$. Putting this into Eq. (2.1), we have

$$\Gamma(1/2) = \int_0^\infty x^{-1/2} e^{-x} dx. \quad (2.6)$$

It may not be immediately clear how to integrate this. For $z = n + 1/2$, it is useful to relate the Gamma function to moments of the Gaussian integral. If we use the substitution $x = y^2$,

$$\begin{aligned} \Gamma\left(n + \frac{1}{2}\right) &= \int_0^\infty x^{(2n-1)/2} e^{-x} dx = \int_0^\infty y^{2n-1} e^{-y^2} (2y dy) \\ &= 2 \int_0^\infty y^{2n} e^{-y^2} dy = \int_{-\infty}^\infty y^{2n} e^{-y^2} dy. \end{aligned} \quad (2.7)$$

A common and useful trick is to introduce a parameter α in the Gaussian, differentiate with respect to this parameter n times, and take $\alpha \rightarrow 1$:

$$\begin{aligned} \int_{-\infty}^\infty y^{2n} e^{-\alpha y^2} dy &= (-1)^n \frac{d^n}{d\alpha^n} \int_0^\infty e^{-\alpha y^2} dy = (-1)^n \frac{d^n}{d\alpha^n} \sqrt{\frac{\pi}{\alpha}} \\ &= (-1)^n \sqrt{\pi} \frac{d^n}{d\alpha^n} \alpha^{-1/2} \\ &= (-1)^n (-1/2)(-1/2-1) \dots (-1/2-(n-1)) \sqrt{\pi} \alpha^{-1/2+n} \\ &= \frac{1}{2} \cdot \frac{3}{2} \dots \frac{2n-1}{2} \sqrt{\pi} \alpha^{-(2n+1)/2} = \frac{(2n-1)!!}{2^n} \sqrt{\pi} \alpha^{-(2n+1)/2}, \end{aligned} \quad (2.8)$$

where we have defined the “double-factorial” as

$$(2n)!! = (2n)(2n-2) \dots (2) \quad (2.9)$$

$$(2n+1)!! = (2n+1)(2n-1) \dots (1). \quad (2.10)$$

Essentially, instead of multiplying consecutive integers one by one, we just multiply integers that are separated by 2 units until we reach either 2 or 1. You can also see that we step n down one unit at a time, which steps $2n$ and $2n+1$ down 2 units.

Taking $\alpha \rightarrow 1$, we finally have

$$\Gamma\left(n + \frac{1}{2}\right) = \frac{(2n-1)!! \sqrt{\pi}}{2^n} = \frac{(2n)! \sqrt{\pi}}{2^{2n} n!}. \quad (2.11)$$

The last equality comes from noticing that we can write

$$\begin{aligned} \frac{(2n)!}{n!} &= \frac{(2n)(2n-1)(2n-2)(2n-3)\dots(3)(2)(1)}{n!} \\ &= \frac{(2n)(2n-2)\dots(2)}{n!} (2n-1)!! \\ &= \frac{2^n(n)(n-1)\dots(2)(1)}{n!} (2n-1)!! = 2^n(2n-1)!! \end{aligned} \quad (2.12)$$

It immediately follows then that

$$\Gamma(1/2) = \sqrt{\pi}. \quad (2.13)$$

This could be gleaned directly from Eq. (2.7) also since $\Gamma(1/2)$ is just the Gaussian integral.

An alternate derivation of this fact is just to exploit the recursion property:

$$\begin{aligned} \Gamma(n+1/2) &= (n-1/2)\Gamma(n-1/2) \\ &= \left(n-\frac{1}{2}\right)\left(n-\frac{3}{2}\right)\dots\left(\frac{3}{2}\right)\left(\frac{1}{2}\right)\Gamma(1/2). \end{aligned} \quad (2.14)$$

This is certainly the more straightforward approach, but the method used above highlights some other useful tools.

Another fact that was thrown at us is the following:

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}. \quad (2.15)$$

If you would like, you can take it as a fact. The proof of this will require a relatively lengthy development, but we will eventually get to the end result. Let us define the beta function

$$B(p, q) = \int_0^1 x^{p-1}(1-x)^{q-1} dx. \quad (2.16)$$

We claim that $B(p, q) = \Gamma(p)\Gamma(q)/\Gamma(p+q)$. Let us now prove this claim. Recall that we can write

$$\Gamma(z) = 2 \int_0^\infty x^{2z-1} e^{-x^2} dx. \quad (2.17)$$

This was shown writing $z = n + 1/2$, but in fact, the transformation did not depend on this assumption – it only lead to our ability to evaluate it in closed form after the substitution. Thus,

$$\Gamma(p)\Gamma(q) = 4 \int_0^\infty \int_0^\infty x^{2p-1} y^{2q-1} e^{-(x^2+y^2)} dx dy. \quad (2.18)$$

Let us change to polar coordinates via $x = r \cos \phi$ and $y = r \sin \phi$

$$\Gamma(p)\Gamma(q) = 4 \int_0^{\pi/2} \cos^{2p-1}(\phi) \sin^{2q-1}(\phi) d\phi \int_0^\infty r^{2p+2q-1} e^{-r^2} dr. \quad (2.19)$$

Note that ϕ only goes from 0 to $\pi/2$ since we only integrate over the first quadrant. Let us look at the angular integral and make the substitution $x = \sin^2 \phi$. Thus, $\cos \phi = \sqrt{1-x}$ and $dx = 2 \sin \phi \cos \phi d\phi$

$$\begin{aligned} \int_0^{\pi/2} \cos^{2p-1}(\phi) \sin^{2q-1}(\phi) d\phi &= \int_0^1 (1-x)^{p-1/2} x^{q-1/2} \frac{dx}{2x^{1/2}(1-x)^{1/2}} \\ &= \frac{1}{2} \int_0^1 x^{q-1} (1-x)^{p-1} dx \\ &= \frac{1}{2} \int_0^1 y^{p-1} (1-y)^{q-1} dy = \frac{1}{2} B(p, q), \end{aligned} \quad (2.20)$$

where in the second-to-last step, we made the substitution $y = 1-x$. Essentially, this substitution showed the reciprocity of the beta function arguments: $B(p, q) = B(q, p)$. Next, it should be clear that the radial integral

$$\int_0^\infty r^{2p+2q-1} e^{-r^2} dr = \frac{1}{2} \Gamma(p+q). \quad (2.21)$$

Putting it all together, we have

$$\Gamma(p)\Gamma(q) = B(p, q)\Gamma(p+q). \quad (2.22)$$

Before we finally prove Eq. (2.15), we have another representation of the beta function. Making the substitution $x = y/(1+y)$, we have $y = x/(1-x)$ and

$$\begin{aligned} B(p, q) &= \int_0^\infty \frac{y^{p-1}}{(1+y)^{p-1}} \frac{1}{(1+y)^{q-1}} \frac{dy}{(1+y)^2} \\ &= \int_0^\infty \frac{y^{p-1}}{(1+y)^{p+q}} dy. \end{aligned} \quad (2.23)$$

Now, we are ready to prove Eq. (2.15). Let $p = z$ and $q = 1-z$. Then, using the most recent representation of the beta function

$$\Gamma(z)\Gamma(1-z) = B(z, 1-z)\Gamma(1) = B(z, 1-z) = \int_0^\infty \frac{x^{z-1}}{1+x} dx. \quad (2.24)$$

We have already evaluated this integral via contour integration. I will evaluate it here again for completeness. We integrate over the contour shown in Fig. 1 with the analytic continuation $x \rightarrow w$:

$$\begin{aligned} 2\pi i(-1)^{z-1} &= \int_{C_{R \rightarrow \infty}} \frac{w^{z-1}}{1+w} dw + \int_\infty^0 \frac{x^{1-z} e^{i2\pi(z-1)}}{1+x} dx \\ &\quad + \int_{C_{\epsilon \rightarrow 0}} \frac{w^{z-1}}{1+w} dw + \int_0^\infty \frac{x^{z-1}}{1+x} dx. \end{aligned} \quad (2.25)$$

The left hand-side is just the residue of the integrand at the pole $w = -1$. Rearranging, we have

$$B(z, 1-z)[1 - e^{i2\pi z}] = -2\pi i e^{i\pi z} - \int_{C_{R \rightarrow 0}} \frac{w^{z-1}}{1+w} dw - \int_{C_{\epsilon \rightarrow 0}} \frac{w^{z-1}}{1+w} dw. \quad (2.26)$$

Along the path C_R , we can write $w = Re^{i\phi}$, giving

$$\int_{C_{R \rightarrow 0}} \frac{w^{z-1}}{1+w} dw = i \int_0^{2\pi} \frac{R^z e^{iz\phi}}{1 + Re^{i\phi}} d\phi. \quad (2.27)$$

Taking $R \Rightarrow \infty$, this is zero, restricting $0 < z < 1$. Recycling most of the work and replacing R with ϵ , it is trivial to see that the integral along the path $C_{\epsilon \rightarrow 0}$ is zero. Thus,

$$\Gamma(z)\Gamma(1-z) = B(z, 1-z) = \frac{-2\pi i e^{i\pi z}}{1 - e^{i2\pi z}} = \pi \frac{2i}{e^{i\pi z} - e^{-i\pi z}} = \frac{\pi}{\sin \pi z}. \quad (2.28)$$

At the moment, it seems that this result only holds for $0 < z < 1$. If we are outside this interval, we can always use the reciprocity relation and find an integer N such that $w = z + n$ is inside the interval $(0, 1)$. Suppose $z > 1$, then there exists $N > 0$ such that $w = z - N$ and

$$\begin{aligned} \Gamma(z)\Gamma(1-z) &= \Gamma(w+N)\Gamma(1-[w+N]) \\ &= (w+[N-1])(w+[N-2]) \dots w \Gamma(w) \\ &\times \frac{1}{1-[w+N]} \frac{1}{2-[w+N]} \dots \frac{1}{N-[w+N]} \Gamma(1-w) \\ &= (-1)^N \Gamma(w)\Gamma(1-w) = (-1)^N \frac{\pi}{\sin \pi w} \\ &= (-1)^N \frac{\pi}{\sin[\pi(z-N)]} = (-1)^N \frac{\pi}{\sin \pi z \cos \pi N} = \frac{\pi}{\sin \pi z} \end{aligned} \quad (2.29)$$

since $\cos \pi N = (-1)^N$. A similar logic can be applied for $z < 0$, so indeed, Eq. (2.15) applies for any complex z .

Appendices

