Contents

0.1 Introduction

$$\text{Linear Algebra} \implies \text{Functional Analysis} \implies \begin{cases} \text{Calculus of Variations} \\ \text{ODEs/PDEs} \\ \text{Approximation Theory} \\ \dots \end{cases}$$

(1) Functional analysis deals with *infinite* dimensional spaces, often spaces of *functions* and certain classes of *mappings* between these spaces.

(2) Can be thought of a (nontrivial) generalization of linear algebra (from finite to infinite dimensional).

(3) The development of functional analytic methods and results are important in various areas of math; in particular they provide a powerful tool for the study of ODEs, PDEs, for example the existence and uniqueness of solutions and the convergence of approximations, etc.

0.2 Linear Algebra

We first draw an analogy between functional analysis and linear algebra, starting from familiar concepts. Let A be a $n \times n$ matrix.

(p1) Given a vector $b \in \mathbb{R}^n$, find $x \in \mathbb{R}^n$ such that $Ax = b$.

Chapter 7

Detour: Quantum Mechanics & Functional Analysis

Beginning of Nov.19, 2021

Consider the system at an arbitrary fixed instant by regarding the time as a parameter which we keep fixed.

In **classical mechanics**, the state is described by specifying position and velocity by a pair of numbers (x, v), whereas in **quantum mechanics**, the state of system is described by a *function*, often times $\psi : \mathbb{R}^n \to \mathbb{C}$.

If we let $\psi \in L^2(\mathbb{R})$ with $\|\psi\|_{L^2} = 1$, then ψ is related to the probability that will be found in a given subset $J \subset \mathbb{R}$ where the probability is

$$\int_J |\psi(q)|^2 \, \mathrm{d}q. \tag{*}$$

(Indeed, we want the particle to always be somewhere on the real line so $\int_{\mathbb{R}} |\psi(q)|^2 \, \mathrm{d}q = 1$.)
Note that (*) is invariant under multiplication by complex numbers with modulus 1, i.e.,

$$\int_J |\psi(q)|^2 \, \mathrm{d}q = \int_J |\alpha\psi(q)|^2 \, \mathrm{d}q \qquad \text{for all } |\alpha| = 1, J \subset \mathbb{R}.$$

Thus, the **deterministic** description of a state in classical mechanics is replaced by a **probabilistic** description of a state in quantum mechanics.

To this end, we define a **state** of our physical system at some instant to be an element $\psi \in L^2(\mathbb{R})$ with $\|\psi\|_{L^2} = 1$, defined uniquely up to multiplication by $\alpha \in \mathbb{C}$ with $|\alpha| = 1$. As said before, $|\psi(q)|^2$ plays a role of a probability density function on $\mathbb{R}$. It follows that we can define the **expected value**, **variance**, and **standard deviation** by

$$\mu_\psi := \int_{\mathbb{R}} q|\psi(q)|^2 \, \mathrm{d}q, \qquad \mathrm{var}_\psi := \int_{\mathbb{R}} (q - \mu_\psi)^2 |\psi(q)|^2 \, \mathrm{d}q, \qquad \text{and} \qquad \mathrm{sd}_\psi := \sqrt{\mathrm{var}_\psi}.$$

(Intuitively, the mean gives the “central location” and the other two show dispersion, just like in probability.)

Note that μ_ψ can be expressed as an inner product:

$$\mu_\psi = \int_{\mathbb{R}} q|\psi(q)|^2 \, \mathrm{d}q = \int_{\mathbb{R}} q\psi(q)\overline{\psi(q)} \, \mathrm{d}q = \langle q\psi(q), \psi(q) \rangle_{L^2}.$$

We can therefore define a **position operator** Q by

$$\mu_\psi(Q) = \langle Q\psi, \psi \rangle = \int_{\mathbb{R}} Q(\psi)\overline{\psi(q)} \, \mathrm{d}q$$

where $Q : \mathfrak{D}(Q) \to L^2(\mathbb{R})$ is defined by $Q\psi(q) = q\psi(q)$. (Note that Q is unbounded, self-adjoint and linear, whose domain for sure includes $C_c^\infty(\mathbb{R})$ and is therefore dense in $L^2(\mathbb{R})$.)

We can also express the variance as an inner product:

$$\mathrm{var}_\psi(Q) = \left\langle (Q - \mu_\psi I)^2 \psi, \psi \right\rangle = \int_{\mathbb{R}} (Q - \mu_\psi I)^2 \psi(q) \overline{\psi(q)}\, \mathrm{d}q.$$

Question. From ψ, how do we obtain some information about quantities that can be observed experimentally? Any such quantity is called an **observable** (e.g., position, momentum, energy).

We have seen that, for "position", we have an available self-adjoint operator Q. This motivates us to define an "observable" of our physical system at some instant to be a general self-adjoint linear operator

$$T : \mathfrak{D}(T) \to L^2(\mathbb{R}) \qquad \text{with } \mathfrak{D}(T) \text{ dense in } L^2(\mathbb{R}).$$

For example, we can define the mean value $\mu_\psi(T)$ by

$$\begin{aligned} \mu_\psi(T) &= \langle T\psi, \psi \rangle = \int_{\mathbb{R}} T\psi(q)\overline{\psi(q)}\, \mathrm{d}q, \\ \mathrm{var}_\psi(T) &= \left\langle (T - \mu_\psi I)^2 \psi, \psi \right\rangle = \int_{\mathbb{R}} (T - \mu_\psi I)^2 \psi(q)\overline{\psi(q)}\, \mathrm{d}q. \end{aligned}$$

Following this path, we get another important observable, the **momentum**, denoted p:

$$D : \mathfrak{D}(D) \to L^2(\mathbb{R}) \qquad \text{defined by} \qquad \psi \mapsto \frac{h}{2\pi i}\frac{\mathrm{d}\psi}{\mathrm{d}q} \tag{Δ}$$

where h is the *Planck's constant* and the domain $\mathfrak{D}(D) \subset L^2(\mathbb{R})$.

A bit of heuristic derivation of (Δ) *using* $E = mc^2$*: suppose a photon has speed* c *and energy* $E = h\nu$ *(*h *Plank constant and* ν *frequency). Then its momentum is by definition* $p = mc = (E/c^2)c = h\nu/c = h/\Lambda = kh/2\pi$ *where* $k = 2\pi/\Lambda$ *and* Λ *is the wavelength* $1/\nu$*.*

Then, by (inverse) Fourier transform,

$$\psi(q) = \frac{1}{\sqrt{h}} \int_{-\infty}^{\infty} \varphi(p) \exp(pq \cdot 2\pi i/h)\, \mathrm{d}p$$

where φ *is the Fourier transform*

$$\varphi(p) = \frac{1}{\sqrt{h}} \int_{-\infty}^{\infty} \psi(q) \exp(pq \cdot (-2\pi i)/h)\, \mathrm{d}q.$$

Physically, this can be interpreted as a representation of ψ *in terms of functions of constant momentum* p *given by* $\psi_p(q) = \varphi(p)e^{ikq} = \varphi(p)\exp(pq \cdot 2\pi i/h)$ *where* $k = 2\pi i/h$ *and* $\varphi(p)$ *is the amplitude. By definition,*

$$|\psi_p(q)|^2 = \psi_p(q)\overline{\psi_p(q)} = \varphi(p)\overline{\varphi(p)} = |\varphi(p)|^2.$$

Since $\|\psi\|_{L^2} = 1$*, we have* $\|\varphi\|_{L^2} = 1$*. We finally define the mean value of the momentum by*

$$\begin{aligned} \tilde{\mu}_\psi &= \int_{-\infty}^{\infty} p|\varphi(p)|^2\, \mathrm{d}p = \int_{-\infty}^{\infty} p\varphi(p)\overline{\varphi(p)}\, \mathrm{d}q \\ &= \int_{-\infty}^{\infty} p\varphi(p)\frac{1}{\sqrt{h}} \int_{-\infty}^{\infty} \overline{\varphi(q)} \exp(pq \cdot 2\pi i/h)\, \mathrm{d}q\, \mathrm{d}p \\ &= \int_{-\infty}^{\infty} \overline{\psi(q)} \int_{-\infty}^{\infty} \varphi(p)\frac{1}{\sqrt{h}} p \exp(pq 2\pi i/h)\, \mathrm{d}p\, \mathrm{d}q \\ [\ldots] &= \int_{-\infty}^{\infty} \frac{h}{2\pi i}\frac{\mathrm{d}\psi(q)}{\mathrm{d}q}\, \mathrm{d}q = \int_{-\infty}^{\infty} \overline{\psi(q)} D\psi\, \mathrm{d}q. \end{aligned}$$

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7.1 The Commutator Operator & the Heisenberg Uncertainty Principle

Let S, T be self-adjoint linear operators with domains in the same complex Hilbert space. Then the operator

$$S := ST - TS$$

is called the **commutator** operator defined on $\mathfrak{D}(C) := \mathfrak{D}(ST) \cap \mathfrak{D}(TS)$.

For example, consider

$$DQ\psi(g) = D(q\psi(g)) = \frac{h}{2\pi i}\left[\psi(q) + q\psi'(q)\right] + \frac{h}{2\pi i}QD\psi(q)$$

so that the commutator $DQ - QD = \frac{h}{2\pi i}I$ defined on its own domain. It is called the **Heisenberg commutator** between position and momentum.

Claim. This domain $\mathfrak{D}(DQ - QD)$ is dense in $L^2(\mathbb{R})$.

Proposition: Lower bound on the commutator

Let S, T be self-adjoint linear operators with domain and range in $L^2(\mathbb{R})$. Then the commutator

$$C := ST - TS$$

satisfies

$$|\mu_\psi(C)| \leqslant 2\mathrm{sd}_\psi(T)\mathrm{sd}_\psi(T) \qquad \text{for all } \psi \in \mathfrak{D}(C).$$

Proof. Write $\mu_1 = \mu_\psi(S)$ and $\mu_2 = \mu_\psi(T)$. Define $A := S - \mu_1 I$ and $\beta := T - \mu_2 I$ on their respective domains. Then $C = ST - TS = AB - BA$ where A, B are both self-adjoint. Then

$$\begin{aligned} \mu_\psi(C) &= \langle (AB - BA)\psi, \psi\rangle \\ &= \langle AB\psi, \psi\rangle - \langle BA\psi, \psi\rangle \\ [\text{self-adjoint}] &= \langle B\psi, A\psi\rangle - \langle A\psi, B\psi\rangle . \end{aligned}$$

Therefore,

$$|\mu_\psi(C)| \leqslant |\langle B\psi, A\psi\rangle| + |\langle A\psi, B\psi\rangle| \leqslant 2\|B\psi\|\|A\psi\|.$$

Note that

$$\|B\psi\| = \sqrt{\langle (T - \mu_2 I)^2\psi, \psi\rangle} = \sqrt{\mathrm{var}_\psi(T)} = \mathrm{sd}_\psi(T)$$

and likewise for $\|A\psi\|$. This completes the proof. □

Theorem: Heisenberg Uncertainty Principle

For the position operator Q and the momentum operator D, $\mathrm{sd}_\psi(D)\mathrm{sd}_\psi(Q) \geqslant \frac{h}{4\pi}$.

Physically, this means that we cannot make a simultaneous measurement of position and momentum of a particle with arbitrary accuracy. More generally, any two observables S and T with nontrivial commutator cannot be simultaneously measured with unlimited precision.

Proof. Recall that $DQ - QD = \frac{h}{2\pi i} I$, so $|\mu_\psi(C)| = \frac{h}{2\pi}$, and the previous proposition gives

$$2\mathrm{sd}_\psi(D)\mathrm{sd}_\psi(Q) \geqslant \frac{h}{2\pi}.$$

□

7.2 Time-Independent Schrödinger Equation

Consider the three-dimensional wave equation

$$\psi_{tt} = \gamma^2 \Delta\psi$$

for $\gamma^2 > 0$ constant and $\Delta\psi := \sum_{i=1}^{3} \frac{\partial^2 \psi}{\partial q_i^2}$. For a simple, time periodic case (stationary waves), we may assume

$$\psi(q_1, q_2, q_3; t) = \psi(q_1, q_2, q_3)e^{-i\omega t}.$$

Then the wave equation reduces to the **Helmholtz** equation

$$\Delta\psi + k^2\psi = 0$$

where $k = \omega/\gamma = 2\pi\nu/\gamma = 2\pi/\Lambda$ where ν is the frequency and Λ the wavelength. We choose $\Lambda = h/mv$ where v is any velocity, the Helmholtz equation can be re-written as

$$0 = \Delta\psi + k^2\psi = \Delta\psi + \frac{8\pi^2 m}{h^2}\frac{mv^2}{2}\psi.$$

Let $E = mv^2/2 + V$ (kinetic and potential) so $mv^2/2 = E - V$. We then obtain the following form of Helmholtz:

$$\Delta\psi + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

or equivalently

$$\left(-\frac{h^2}{8\pi^2 m}\Delta + V\right)\psi = E\psi. \tag{*}$$

Both forms are called the **time-independent Schrödinger equation**. From a mathematical viewpoint, possible energy levels of the system will depend on the spectrum of the operator defined by the LHS of (*).