Mathematical Foundations of Quantum Mechanics

From Functional Analysis to Quantum Computing

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Boston University Directed Reading Program

Introduction

- Sophomore undergraduate studying math and computer science at Boston University
- Interested in quantum computing and mechanics as well as a multitude of different mathematical subjects
- Wanted to explore the mathematical foundations of certain quantum formulas & algorithms normally glossed over in other classes

Basics of Functional Analysis: Inner Product

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If $\mathscr{X}$ is a vector space in the complex field $\mathbb{C}$, an inner product (denoted $\langle \cdot, \cdot \rangle$ or $\langle \cdot | \cdot \rangle$) for all $\alpha, \beta \in \mathbb{C}$ and $x, y, z \in \mathscr{X}$ satisfies the following:

- $\langle \alpha x + \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle$
- $\langle x, \alpha y + \beta z \rangle = \overline{\alpha} \langle x, y \rangle + \overline{\beta} \langle x, z \rangle$
- $\langle x, x \rangle \geq 0$
- $\langle x, y \rangle = \langle y, x \rangle$
- $\langle x, 0 \rangle = \langle 0, y \rangle = 0$
- If $\langle x, x \rangle = 0$, then $x = 0$

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The key thing to note is that these properties all apply to the dot product for finite dimensions.

Basics of Functional Analysis: Introducing L2

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We use L^2 since it has a lot of nice mathematical and physical properties, one of which is that it behaves a lot like $\mathbb{R}^n$ in infinite dimensions.

Schrödinger Equation: Infinite Square Well

The Schrödinger equation states that

$$\begin{aligned} i\hbar\frac{\partial \Psi}{\partial t}(t,x) &= -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}(t,x) + V(x)\Psi(t,x) \\ &= H\Psi(t,x) \end{aligned}$$

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If we assume that time is independent, i.e. $\Psi(t,x) = \varphi(t)\psi(x)$, then we can separate this equation and solve

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The potential of the infinite square well is described by

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

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We can let $H : L^2[0, a] \to L^2[0, a]$ with $\psi(0) = \psi(a) = 0$. In this case, we know that $H = -\frac{\hbar^2}{2m}\partial_{xx}$ in $[0, a]$. If we solve the ODE $-\frac{\hbar^2}{2m}\psi_{xx} = E\psi$, we find that the eigenvalues and eigenfunctions are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2},\ \psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\ \text{for } n = 1, 2, 3, \dots$$

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These $\{\psi_n\}_{n=1}^{\infty}$ form an orthonormal basis of $L^2[0, a]$, so

$$\Psi(t, x) = \sum_{n=1}^{\infty}\langle\Psi(0, \cdot), \psi_n\rangle e^{-i\frac{E_n}{\hbar}t}\psi_n(t)$$

Therefore, we have solved the Schrödinger equation for the infinite square well case.

Schrödinger Equation: Free Particle

Let's now suppose that $V(x) = 0$. Our previous strategy was to solve the ODE $-\frac{\hbar^2}{2m}\psi_{xx} = E\psi$ and find an orthonormal eigenbasis $\{\psi_n\}$ with eigenvalues $\{E_n\}$ on $L^2([0, a])$, so we could write a solution as a linear combination.

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However, with no boundary, any E will work here. We want to ultimately write

$$\Psi(t, x) = \sum_{n=1}^{\infty} \langle \Psi(0, \cdot), \psi_n \rangle e^{-i\frac{E_n}{\hbar}t} \psi_n(t)$$

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How can we do this? We can use the continuous version of summation $\implies$ integration!

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Let $f \in L^2[0, 2\pi]$ and $e_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, which can be thought of as a period $\frac{2\pi}{k}$ "frequency". We can see that

$$f_n = \int_0^{2\pi} f(x) e_k(x)\, dx \implies f(x) = \sum_{n=0}^{\infty} f_n e_n(x) = \sum_{n=0}^{\infty} \langle f, e_n \rangle e_n(x)$$

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Since k can be any real number, we write this as an integral:

$$\Psi(t, x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar}{2m} k^2 t)}\, dk$$

Continuous Fourier Transform

The Fourier transform is defined as

$$\widehat{f}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-i\xi x}\, dx \text{ for } \xi \in \mathbb{R}$$

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We can invert the Fourier transform very easily. With $\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$, we have an inversion formula

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A few other nice properties:

- Maps derivatives to products: $\widehat{f^{(n)}}(\xi) = (i\xi)^n \widehat{f}(\xi)$
- Maps products to convolutions: $\mathcal{F}(fg)(\xi) = (\widehat{f} * \widehat{g})(\xi)$
- Maps convolutions to products: $\mathcal{F}(f * g)(\xi) = \widehat{f}(\xi)\widehat{g}(\xi)$

Discrete Fourier Transform

Given data $(x_0, x_1, \ldots, x_{N-1}) \in \mathbb{C}^{N-1}$, we want to form $(y_0, y_1, \ldots, y_{N-1}) \in \mathbb{C}^{N-1}$ where $y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \omega_N^{-jk}$ and $\omega_N := e^{i\frac{2\pi}{N}}$. This is a discrete variation of the Fourier transform we just defined.

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In quantum computing, the inverse of this operation is known as the quantum Fourier transform. If we have a quantum state $|x\rangle = \sum_{j=0}^{N-1} x_j |j\rangle$, the QFT maps $|x\rangle \mapsto |y\rangle = \sum_{k=0}^{N-1} y_k |k\rangle$, where $y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \omega_N^{jk}$.

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The QFT can be thought of as a unitary matrix mapping

$$F_N = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega_N & \omega_N^2 & \cdots & \omega_N^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega_N^{N-1} & \omega_N^{2(N-1)} & \cdots & \omega_N^{(N-1)(N-1)} \end{bmatrix}$$

Quantum Phase Estimation

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Assume that $\theta = 2\pi j/2^m$ for some integer j. Then, we know the inverse QFT maps

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In fact, regardless of the value of θ, the output $|j\rangle$ turns out to be a very good approximation.

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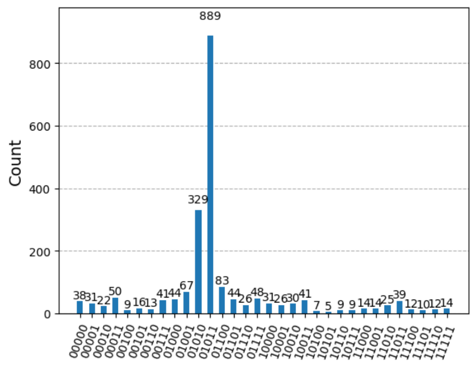
We then discard the $|v_\theta\rangle$ register. We can then simply apply the inverse QFT to get an output $|j\rangle$ such that $\theta \approx 2\pi j/2^m$.

QPE Example

Given this real quantum output plot, what can we say about θ?



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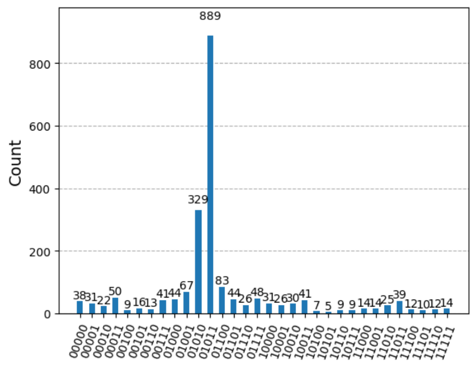

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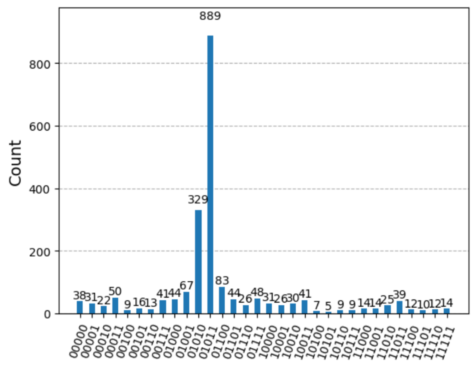

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In fact, the actual $\theta = 2\pi/3$.

Thank you for listening!

Let me know if you have any questions!