Spectral Decomposition of Quantum-Mechanical Operators

Tuesday, May 2, 2017

Daniel Halmrast
Advisor: Dr. David Gaebler

Outline

What Is a Hilbert Space?

A *Hilbert space* is an inner product space that is complete with respect to the induced metric $d(x,y) = \langle x-y, x-y \rangle$.

Example

1. $\mathbb{C}^n$ with the inner product $\langle x, y \rangle = x \cdot y$
2. $L^2(X, \mu)$ with the inner product $\langle f, g \rangle = \int_X f\overline{g} d\mu$ (Riesz-Fischer)

$L^2(X, \mu)$

$L^2(X, \mu)$ is the set of all square-integrable functions from X to $\mathbb{C}$ under the equivalence relation

$$f \sim g \iff \int_X |f - g|^2 d\mu = 0$$

$L^2(X,\mu)$

$L^2(X,\mu)$ is the set of all square-integrable functions from X to $\mathbb{C}$ under the equivalence relation

$$f \sim g \iff \int_X |f-g|^2 d\mu = 0$$

Example

$L^2(\mathbb{R}, dx)$ is the L^2 space of functions on the real number line.

- The characteristic function $\chi_{[0,1]}(x)$ is a square-integrable function with integral 1.
- The complex exponential e^{ikx} is not square-integrable on the real number line, and is thus not part of $L^2(\mathbb{R}, dx)$.

Operators in Hilbert Spaces

- A *linear operator* on a Hilbert space $\mathbf{H}$ is a function $T : \mathbf{H} \to \mathbf{H}$ that satisfies $T(\alpha x_1 + \beta x_2) = \alpha T(x_1) + \beta T(x_2)$ for $x_1, x_2 \in \mathbf{H}$.
- A linear operator is *bounded* if there exists some scalar C such that $\forall x \in \mathbf{H} : ||T(x)|| \leq C||x||$

Operators in Hilbert Spaces

- A *linear operator* on a Hilbert space $\mathbf{H}$ is a function $T : \mathbf{H} \to \mathbf{H}$ that satisfies $T(\alpha x_1 + \beta x_2) = \alpha T(x_1) + \beta T(x_2)$ for $x_1, x_2 \in \mathbf{H}$.
- A linear operator is *bounded* if there exists some scalar C such that $\forall x \in \mathbf{H} : ||T(x)|| \leq C||x||$

Fun fact: bounded linear operators are the morphisms in the category of Hilbert spaces.

Operators in Hilbert Spaces

- A *linear operator* on a Hilbert space $\mathbf{H}$ is a function $T : \mathbf{H} \to \mathbf{H}$ that satisfies $T(\alpha x_1 + \beta x_2) = \alpha T(x_1) + \beta T(x_2)$ for $x_1, x_2 \in \mathbf{H}$.
- A linear operator is *bounded* if there exists some scalar C such that $\forall x \in \mathbf{H} : ||T(x)|| \leq C||x||$

Fun fact: bounded linear operators are the morphisms in the category of Hilbert spaces.

Example

1. Any matrix $M \in \mathbb{C}^{n \times n}$ is a bounded linear operator on $\mathbb{C}^n$.
2. Given a subspace $M \subset \mathbf{H}$, the orthogonal projection operator P_M is a bounded linear operator on $\mathbf{H}$.
3. for any essentially bounded function ϕ on a measure space (X, μ), the multiplication operator M_ϕ, given by $M_\phi(f) = \phi f$ is a bounded linear operator on $L^2(X, \mu)$.

Adjoints and Normality

The *adjoint* of an operator A on a Hilbert space $\mathbf{H}$ is the unique operator A^* that satisfies

$$\langle Ax, y \rangle = \langle x, A^* y \rangle$$

for all x, y in $\mathbf{H}$. An operator is said to be *normal* if it commutes with its adjoint, and *self-adjoint* if it equals its own adjoint.

Example

1. The adjoint of a matrix $M \in \mathbb{C}^{n \times n}$ is the conjugate transpose $M^\dagger$.
2. The projection operator P_M is self-adjoint.
3. The adjoint of the multiplication operator M_ϕ is multiplication by the conjugate $M_{\overline{\phi}}$.

The Spectrum of an Operator

In finite dimensions, the spectrum of a matrix M is the set of eigenvalues for that matrix (i.e. the set of all λ such that $(A - \lambda I)x = 0$ for some x).
In infinite dimensions, however, there are more ways to fail invertibility than just having a nontrivial kernel.

Definition

The *spectrum* of an operator A, denoted $\sigma(A)$, is the set of all complex numbers λ for which the operator $A - \lambda I$ is not invertible.

The Spectral Partition

Question

In what ways can $A - \lambda I$ *fail to be invertible?*

The Spectral Partition

Question

In what ways can $A - \lambda I$ fail to be invertible?

1. $A - \lambda I$ has nontrivial kernel (the *point spectrum*).

The Spectral Partition

Question

In what ways can $A - \lambda I$ fail to be invertible?

1. $A - \lambda I$ has nontrivial kernel (the *point spectrum*).
2. $A - \lambda I$ is not bounded below (the *approximate point spectrum*).

The Spectral Partition

Question

In what ways can $A - \lambda I$ fail to be invertible?

1. $A - \lambda I$ has nontrivial kernel (the *point spectrum*).
2. $A - \lambda I$ is not bounded below (the *approximate point spectrum*).
3. $A - \lambda I$ does not have dense range (the *compression spectrum*).

Interpreting the Approximate Point Spectrum

For an operator $A - \lambda I$ to *not* be bounded below, there must exist some sequence $\{h_n\}$ of unit vectors such that

$$||(A - \lambda I)h_n|| \to 0$$

Theorem

If A_n is a sequence of invertible operators that converge to $A - \lambda I$, where $A - \lambda I$ is not invertible, then $\lambda \in \sigma_{AP}(A)$.

Theorem

$\overline{\sigma_P(A)} \subset \sigma_{AP}(A)$, where $\overline{\sigma_P(A)}$ is the closure of the point spectrum of A.

Examples

Example

In finite dimensions, $\sigma(M) = \sigma_P(M)$. That is, the spectrum is entirely a point spectrum.

Example

The infinite matrix $M = \begin{bmatrix} 1 & 0 & \cdots & 0 & \cdots \\ 0 & \frac{1}{2} & \cdots & 0 & \cdots \\ \vdots & \vdots & \ddots & 0 & \cdots \\ 0 & 0 & 0 & \frac{1}{2^n} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$

has $\sigma_P(M) = \{\frac{1}{2^n}\}$ and $\sigma_{AP}(M) = \sigma_P(M) \cup \{0\}$.

Examples

Example

Consider the operator $M_x : f(x) \mapsto xf(x)$ on the Hilbert space $L^2([0,1], dx)$.

- For $\lambda \notin [0,1]$, the operator of multiplication by $\frac{1}{x-\lambda}$ inverts $(M_x - \lambda I)$.
- For $\lambda \in [0,1]$, the operator has no inverse.
- Furthermore, each $\lambda \in [0,1]$ is part of $\sigma_{AP}(M_x)$.

$$\{f_n(x)\}_\lambda = \begin{cases} n & \text{if } x \in V_{\frac{1}{n^2}}(\lambda) \\ 0 & \text{else} \end{cases}$$

The Spectral Theorem for Matrices

Theorem (The Spectral Theorem–Finite Dimension)

Every normal matrix A is unitarily equivalent to a diagonal matrix. That is, $A = UDU^*$ for some unitary matrix U and some diagonal matrix D.

Here, the unitary matrix has columns equal to the eigenvectors of A, and the diagonal matrix has the corresponding eigenvalues of A.

The Spectral Theorem for Matrices (Cot'd)

Alternately,

Theorem (The Spectral Theorem–Finite Dimension, Take Two)

Every normal matrix A is expressable as a linear combination of projections onto its eigenspaces. That is,

$$A = \sum_{i=1}^{n} \lambda_i P_{\lambda_i}$$

where $\{\lambda_i\}$ is the spectrum of A, and P_{λ_i} is an orthogonal projection onto the eigenspace associated with λ_i.

Measures

Extending to infinite dimensions gets tricky, we'll need the idea of a measure to continue...

Measures

Extending to infinite dimensions gets tricky, we'll need the idea of a measure to continue...

A *measure* on a space X is a function $\mu : P[X] \to \mathbb{R}_+ \cup \{\infty\}$ where:

- $\mu(\emptyset) = 0$
- $\mu(A \cup B) = \mu(A) + \mu(B)$ for A, B disjoint sets

Measures

Extending to infinite dimensions gets tricky, we'll need the idea of a measure to continue...

A *measure* on a space X is a function $\mu : P[X] \to \mathbb{R}_+ \cup \{\infty\}$ where:

- $\mu(\emptyset) = 0$
- $\mu(A \cup B) = \mu(A) + \mu(B)$ for A, B disjoint sets

Intuitively: μ measures the "weight" of a set.

Measures

Extending to infinite dimensions gets tricky, we'll need the idea of a measure to continue...

A *measure* on a space X is a function $\mu : P[X] \to \mathbb{R}_+ \cup \{\infty\}$ where:

- $\mu(\emptyset) = 0$
- $\mu(A \cup B) = \mu(A) + \mu(B)$ for A, B disjoint sets

Intuitively: μ measures the "weight" of a set.

Practically: μ allows us to integrate (the Lebesgue Integral).

Measures: Examples

Example

$X = \mathbb{R}$, and $d\mu = dx$ leads to the standard measure on the real number line: $\mu([a,b]) = b - a$. Here, the integral is the standard integral

$$\int_{\mathbb{R}} f(x)dx$$

Measures: Examples

Example

$X = \mathbb{R}$, and $d\mu = dx$ leads to the standard measure on the real number line: $\mu([a, b]) = b - a$. Here, the integral is the standard integral

$$\int_{\mathbb{R}} f(x) dx$$

Example

$X = \mathbb{N}$, and $d\mu$ is the counting (δ) measure $\mu(S) = |S|$. The integral, then, is

$$\int_{\mathbb{N}} f(n) d\mu = \sum_{i=1}^{\infty} f(n)$$

The Spectral Theorem for Operators

What happens when we extend to the infinite-dimensional case?

Theorem (The Spectral Theorem–Projection-valued Measures)

Every normal operator A on a Hilbert space $\boldsymbol{H}$ is expressible as

$$A = \int_{\sigma(A)} z dE(z)$$

Where dE is a projection-valued measure *on the spectrum of A.*

Examples

Example

Let $M = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \lambda_n \end{bmatrix}$
Then, the spectral measure $E(S)$ is the δ-measure on $\sigma(M)$ with $E(\lambda_i) = P_{\lambda_i}$, and the spectral theorem states that

$$M = \int_{\sigma(M)=\{\lambda_i\}} z dE(z) = \sum_{i=1}^{n} \lambda_i P_{\lambda_i}$$

which is a restatement of the familiar spectral theorem.

Example: Multiplication

Example

Let M_x be the familiar multiplication operator on $L^2([0, 1], dx)$. We have seen already that $\sigma(M_x) = \sigma_{AP}(M_x) = [0, 1]$. The spectral measure $E(S)$ for an interval S is given as M_{χ_S} for χ_S the indicator function on S.

$$M_x = \int_{\sigma(M_x)} z dE(z)$$

Example: Multiplication

Example

Let M_x be the familiar multiplication operator on $L^2([0,1], dx)$.
We have seen already that $\sigma(M_x) = \sigma_{AP}(M_x) = [0,1]$.
The spectral measure $E(S)$ for an interval S is given as M_{χ_S} for χ_S the indicator function on S.

$$M_x = \int_{\sigma(M_x)} z dE(z)$$

Question

What is $dE(z)$?

What is $dE(z)$?

Motivation: $Ax = \lambda x$, the eigenvalue equation.

$$\begin{aligned} M_x f &= \lambda f \\ x f(x) &= \lambda f(x) \\ \implies f(x) &= 0 \text{ for } x \neq \lambda \end{aligned}$$

What is $dE(z)$?

Motivation: $Ax = \lambda x$, the eigenvalue equation.

$$M_x f = \lambda f$$
$$xf(x) = \lambda f(x)$$
$$\implies f(x) = 0 \text{ for } x \neq \lambda$$

$f(x) = \delta_\lambda(x)$?

More on this later...

Alternative Approach: Direct Integrals

Given a measure space (X, μ) and a collection of separable Hilbert spaces $\{\mathbf{H}_\lambda\}_{\lambda \in X}$ with a measureability structure, the *direct integral*

$$\int_X^{\oplus} \mathbf{H}_\lambda d\mu(\lambda)$$

is the space of equivalence classes of sections s for which $||s|| < \infty$ under the norm induced from the inner product

$$\langle s_1, s_2 \rangle = \int_X \langle s_1(\lambda), s_2(\lambda) \rangle d\mu(\lambda)$$

The Spectral Theorem–Direct Integral

Theorem

Given a normal operator A, there exists a σ-finite measure μ on $\sigma(A)$ such that A is unitarily equivalent to the multiplication operator M_λ on the direct integral

$$\int_{\sigma(A)}^{\oplus} \boldsymbol{H}_\lambda d\mu(\lambda)$$

The $\mathbf{H}_\lambda$ can be thought of as the "generalized eigenspaces" of the operator, and the measure will count their "generalized multiplicity". (Remember the $\delta(x)$?)

Quantum Lives in a Hilbert Space

Quantum Mechanics has five basic "axioms" to describe the theory.

1. Associated with each quantum system is a Hilbert space, and quantum states are unit vectors in this Hilbert space.
2. Each classical phase space variable has an associated self-adjoint operator known as a quantum observable.
3. The probability distribution of an observable $\hat{f}$ for a quantum state ψ satisfies $\langle f \rangle = \langle \psi, \hat{f}\psi \rangle$
4. If an observable $\hat{f}$ is measured to have a value of λ for a quantum system with initial state ψ, it will collapse to a state ψ' satisfying $\hat{f}\psi' = \lambda\psi'$
5. Time evolution is governed by the Schrodinger equation

$$\partial_t \psi - \frac{1}{i\hbar}\hat{H}\psi$$

Quantization of Energy

Proposition

The quantization of the phase space variables x and p are

- $x \to M_x$
- $p \to -i\hbar\frac{d}{dx}$

Example

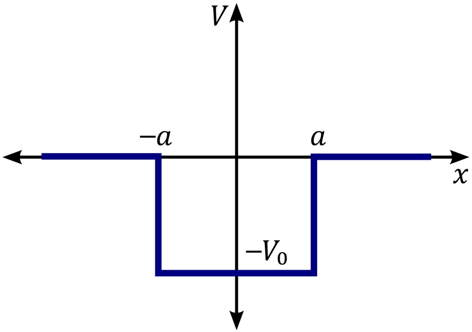
The standard quantization of kinetic energy uses the identity

$$KE = \frac{p^2}{2m}$$

Which implies that

$$\hat{KE} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

The Finite Square Well



The Finite Square Well

The Hilbert space for the finite square well can be taken to be $L^2(\mathbb{R})$, and the Hamiltonian for the finite square well is

$$\hat{H}(x) = \begin{cases} \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} - V_0 & \text{if } x \in [-a, a] \\ \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} & \text{else} \end{cases}$$

The goal is to find the *allowed energies* for this system. To do so, we need to find the spectrum of $\hat{H}$.

The Finite Square Well: Results

First pass: solve $\hat{H}\psi = E\psi$ to find eigenvalues. As it turns out, this splits into two cases: $V_0 < E < 0$ and $E > 0$.

Result

- *For $V_0 < E < 0$, the solutions are of the form*

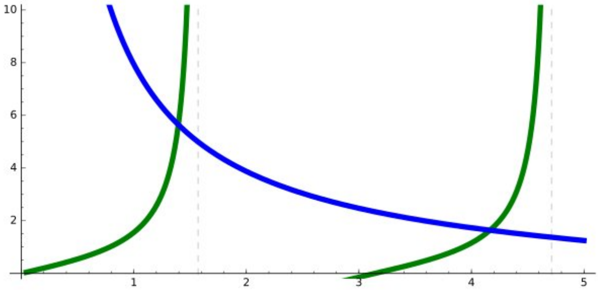
$$\psi(x) = \begin{cases} C_1 e^{\sqrt{\epsilon} x} & \text{if } x \in (-\infty, -a] \\ C_2 \cos(\sqrt{v - \epsilon}) & \text{if } x \in [-a, a] \\ C_3 e^{-\sqrt{\epsilon} x} & \text{if } x \in [a, \infty) \end{cases}$$

  with the condition that $\sqrt{\epsilon} = \sqrt{v - \epsilon} \tan(\sqrt{v - \epsilon} a)$

- *For $E > 0$, the solutions are linear combinations of* $\psi_E(x) = C_1 e^{ikx} + C_2 e^{-ikx}$ *for* $k = \frac{\sqrt{2mE}}{\hbar}$.

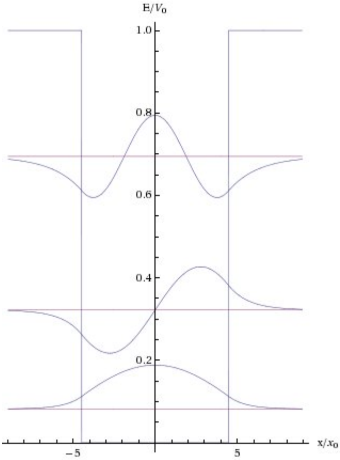
The Finite Square Well: Bound states

For $E < V_0$, we find a finite discrete set of allowed energies.



$$\sqrt{\epsilon} = \sqrt{v - \epsilon}\tan(\sqrt{v - \epsilon}a)$$

The Finite Square Well: Bound States(Cot'd)



The Finite Square Well: Spectral Partitions

Each bound state corresponds to an energy in the point spectrum $\sigma_P(\hat{H})$, and each free state corresponds to an energy in the approximate point spectrum $\sigma_{AP}(\hat{H})$.

Proof.

For $E > 0$, let ψ solve $\hat{H}\psi = E\psi$, and define a sequence of functions

$$\psi_n(x) = \psi * \begin{cases} 0 & |x| \geq n+1 \\ 1 & |x| \leq n \\ \chi_{[0,\frac{1}{3}]}(-x-n) & -(n+1) < x < -n \\ \chi_{[0,\frac{1}{3}]}(x-n) & n < x < n+1 \end{cases}$$

Then, it can be shown that $lim_{n\to\infty} \frac{||(\hat{H}-EI)\psi_n||}{||\psi_n||} = 0$. $\square$

The Finite Square Well: Projection-Valued Measure

For this slide, E will represent an element of the spectrum of $\hat{H}$, and F will be a projection-valued measure.

- For the point spectrum,

$$dF(E) = P_E$$

  where P_E is the orthogonal projection onto the one dimensional subspace of the state with energy E.

- For the approximate point spectrum, one can interpret $dF(E)$ to be a projection onto the two dimensional subspace spanned by the "states"

$$\psi_E(x) = e^{-ikx}$$
$$\psi_E(x) = e^{ikx}$$

The Finite Square Well: Projection-Valued Measure (Cot'd)

Problem:

$$\psi_E(x) = e^{-ikx}$$
$$\psi_E(x) = e^{ikx}$$

is not in $L^2(\mathbb{R})$!

The Finite Square Well: Projection-Valued Measure (Cot'd)

Problem:

$$\psi_E(x) = e^{-ikx}$$
$$\psi_E(x) = e^{ikx}$$

is not in $L^2(\mathbb{R})$!

This is because $\mu(E) = 0$...

The Finite Square Well: Projection-Valued Measure (Cot'd)

Problem:

$$\psi_E(x) = e^{-ikx}$$
$$\psi_E(x) = e^{ikx}$$

is not in $L^2(\mathbb{R})$!
This is because $\mu(E) = 0$...
For a set of positive measure (e.g. an interval of energies), we get infinitely many frequencies to work with, and can build a square-integrable function from them!

Example

For an interval of energies $k \in [1, 2]$, the state

$$\psi(x) = \int_{[1,2]} \chi_{[1,2]}(x) e^{ikx} dk$$

is a square-integrable solution!

The Finite Square Well: Direct Integral

The spectrum of $\hat{H}$ is $\sigma(\hat{H}) = E_n \cup (0, \infty)$ for some finite set of allowed bound energies E_n.

The measure on the point spectrum is the counting measure, so that part of the integral becomes

$$\int_{\sigma_P(\hat{H})}^{\oplus} \mathbf{H}_E d\mu(E) = \oplus_{i=1}^{n} \mathbf{H}_E$$

Where $\mathbf{H}_E$ is the one dimensional subspace of the state with energy E.

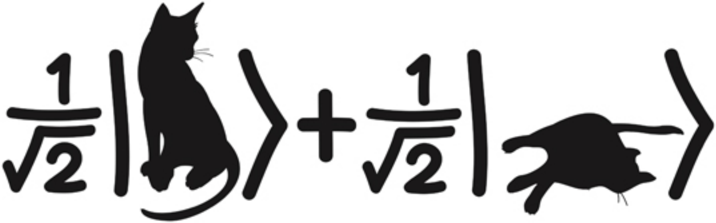
The Finite Square Well: Direct Integral

The measure on the approximate point spectrum is more mysterious, but the integrand $\mathbf{H}_E$ can be shown to be the two-dimensional subspace of complex exponentials e^{ikx} and e^{-ikx}. Thus, the Hilbert space for which $\hat{H}$ acts as multiplication is

$$\oplus_{i=1}^{n} \mathbf{H}_{E_n} \oplus \int_{\sigma_{AP}(\hat{H})}^{\oplus} H_E d\mu(E)$$

Conclusions

- The spectral theorem still works in infinite dimensions.
- Infinite dimensions potentially leads to a continuous spectrum.
- This is fixed by introducing an integral across the more generalized eigenspaces, either on projections (PVM) or on the space itself (DI).
- Spectral partitions help with understanding which parts of the spectrum will be continuous or not.
- These formulations provide a new perspective on some key results in quantum mechanics



Special thanks to Dr. Gaebler,
The Hillsdale College Mathematics Department,
And viewers like you!