

# Formalism of quantum mechanics from the point of view of machine learning

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## Informal Introduction

Suppose that we want to describe nature probabilistically in terms of some probability distribution  $\rho(x, t)$ . To predict future state we may have some evolution equation

$$\frac{\partial \rho(x, t)}{\partial t} = F(\rho(x, t)) \quad (1)$$

We know that for all  $t$  our probability distribution is normalized

$$\int \rho(x, t) dx = 1 \quad \forall t \quad (2)$$

## Informal Introduction

Could we interpret this normalization condition

$$\int \rho(x, t) dx = 1 \quad \forall t \quad (3)$$

in terms of  $L_2$  norm on a space of smooth functions?

$$\int |\sqrt{\rho(x, t)}|^2 dx = \|\sqrt{\rho(x, t)}\|_{L_2}^2 = 1 \quad \forall t \quad (4)$$

If we want our probability density  $\rho(x, t)$  to be real-valued then we have to assume that in general  $\sqrt{\rho(x, t)}$  may have some complex phase and it will not affect our observations of average statistics of the distribution  $\rho(x, t)$

$$\sqrt{\rho(x, t)} \rightarrow \sqrt{\rho(x, t)} e^{iS(x, t)} \quad (5)$$

## Informal Introduction

Then the normalization condition

$$\int \rho(x, t) dx = 1 \quad \forall t \quad (6)$$

becomes

$$\begin{aligned} \|\sqrt{\rho(x, t)} e^{iS(x, t)}\|_{L_2} &= \int \left( \sqrt{\rho(x, t)} e^{iS(x, t)} \right)^* \sqrt{\rho(x, t)} e^{iS(x, t)} dx = \\ &= \int \sqrt{\rho(x, t)} e^{-iS(x, t)} \sqrt{\rho(x, t)} e^{iS(x, t)} dx = \\ &= \int \rho(x, t) dx = 1 \end{aligned}$$

so we could interpret the **state** of the system as a **unit vector** in a Hilbert space of functions

$$\psi(x, t) = \sqrt{\rho(x, t)} e^{iS(x, t)} \quad (7)$$

# Informal Introduction

## Note about Hilbert spaces:

- ▶ Hilbert space  $\mathcal{H} \rightarrow$  vector space with inner product;

$$\langle ., . \rangle : \mathcal{H} \otimes \mathcal{H} \rightarrow \mathbb{C}$$

- ▶ inner product  $\rightarrow$  metric;

$$d(x, y) = \sqrt{\langle x - y, x - y \rangle}$$

- ▶ Hilbert space is a complete metric space = every Cauchy sequence is convergent
- ▶ Hilbert space is separable = there is a countable basis

$$\forall f \in \mathcal{H} : f = \sum_{i=1}^{\infty} \langle f, f_n \rangle f_n, \quad \langle f_m, f_n \rangle = \delta_{n.m}$$

**Note about terminology:** in physics Hilbert spaces can be finite-dimensional

## Informal Introduction

The **state** of the system is a **unit vector** in a Hilbert space of functions

$$\psi(x, t) = \sqrt{\rho(x, t)} e^{iS(x, t)} \quad (8)$$

What can we say about the evolution equation

$$\frac{\partial \rho(x, t)}{\partial t} = F(\rho(x, t)) \quad (9)$$

in terms of  $\psi(x, t)$ ?

Assume that evolution is described by an action of some operator  $L : \mathcal{H} \rightarrow \mathcal{H}$  on the Hilbert space  $\mathcal{H}$

$$\psi(x, t') = L[\psi(x, t)] \quad (10)$$

What are the properties of  $L$ ?

## Informal Introduction

Assume that evolution is described by an action of some operator  $L : \mathcal{H} \rightarrow \mathcal{H}$  on the Hilbert space  $\mathcal{H}$

$$\psi(x, t') = L[\psi(x, t)] \quad (11)$$

What are the properties of  $L$ ?

1)  $L$  doesn't change the norm of the vector  $\psi(x, t)$ . It means that  $L$  only can rotate  $\psi(x, t)$  in the Hilbert space.

**Real case:** real rotation represented by a matrix from the orthogonal group  $O^T O = I$

**Complex case:** complex rotation represented by a matrix from the unitary group  $U^\dagger U = I$ , where  $U^\dagger = (U^T)^*$  - Hermitian conjugate.

**Evolution operator has to be unitary.**

## Informal Introduction

- ▶ Evolution operator  $L$  have to be unitary.

$$\psi(x, t') = L[\psi(x, t)] \quad (12)$$

- ▶ If  $\psi(x, t + dt)$  and  $\psi(x, t)$  are close for small  $dt$  the evolution operator should be close to unity.
- ▶ Unitary operators form a Lie group. Near the group identity every element of a Lie group = exponent of Lie algebra.
- ▶ Lie group = manifold with a group structure
- ▶ Lie algebra = tangent space at the group identity equipped with a Lie bracket (commutator)

For  $g$  from the Lie algebra of the Unitary group

$$L = e^g \quad (13)$$



# Informal Introduction

## Example of Lie group: 1d translations

Consider Taylor expansion

$$f(x + a) = \sum_{n=0}^{\infty} \frac{1}{n!} \left( a \frac{d}{dx} \right)^n f(x) = e^{a \frac{d}{dx}} f(x)$$

From the group-theoretic point of view we have representation of the Lie group of 1d translations on the  $\infty$ -dimensional space of functions: translation from  $x$  to  $x + a$  corresponds to the multiplication of a function  $f$  by an operator  $e^{a \frac{d}{dx}}$ .

Usually say that operator  $e^{a \frac{d}{dx}}$  is a representation of an element  $a \in (\mathbb{R}, +)$  from the Lie group of 1d translations.

## Informal Introduction

### Example of Lie group: 1d translations

Consider Taylor expansion

$$f(x + a) = e^{a \frac{d}{dx}} f(x)$$

Usually say that operator  $e^{a \frac{d}{dx}}$  is a **representation** of an element  $a \in (\mathbb{R}, +)$  from the Lie group of 1d translations.

**Note:** "representation" = linear map  $T: \{\text{group}\} \rightarrow \{\text{linear operators on a vector space}\}$ , which maps group multiplication to the composition of linear operators, i. e.

$$T(g_1 \times g_2) = T(g_1) \circ T(g_2).$$

**In this particular example:**  $T$  is an operator on the space of smooth functions

$$T(a) = e^{a \frac{d}{dx}}$$

$$T(a) \circ T(b) = e^{a \frac{d}{dx}} e^{b \frac{d}{dx}} = \left| \frac{d}{dx} \text{commutes with itself} \right| =$$

$$= e^{(a+b) \frac{d}{dx}} = T(a + b)$$

# Informal Introduction

## Example of Lie group: 1d translations

$$f(x + a) = e^{a \frac{d}{dx}} f(x)$$

Lie group:  $e^{a \frac{d}{dx}}$

Lie algebra:  $a \frac{d}{dx}$

Differential operator  $\frac{d}{dx}$  forms basis of the corresponding Lie algebra, so the Lie algebra of translations in  $\infty$ -dimensional representation consists of elements of the form  $a \frac{d}{dx}$ ,  $a \in \mathbb{R}$ .

# Informal Introduction

## Back to the evolution operator = operator of time translations

Denote by the  $L_{t,t'}$  operator which transforms the state  $\psi(x, t)$  to the state  $\psi(x, t')$ . We know that

$$L_{t,t} = I \quad (14)$$

and that

$$L_{t,t'} \cdot L_{t',t''} = L_{t,t''} \quad (15)$$

In the last formula  $\cdot$  represents a multiplication of the unitary group which is the composition of operators.

From the point of view of Lie algebra

$$L_{t,t} = I \rightarrow e^{g(t,t')} = e^0 \quad (16)$$

$$L_{t,t'} \cdot L_{t',t''} = L_{t,t''} \rightarrow e^{g(t,t') + g(t',t'')} = e^{g(t,t'')} \quad (17)$$

# Informal Introduction

From the point of view of Lie algebra

$$L_{t,t} = I \rightarrow e^{g(t,t')} = e^0$$

$$L_{t,t'} \cdot L_{t',t''} = L_{t,t''} \rightarrow e^{g(t,t') + g(t',t'')} = e^{g(t,t'')}$$

We can choose

$$g(t, t') = (t - t')iH$$

where  $H$  is a Hermitian operator:  $H^\dagger = H$

**Proposition** If  $H$  is a Hermitian operator then  $L = e^{(t-t')iH}$  is a unitary operator.

**Proposition** Hermitian operators have real eigenvalues.

## Informal Introduction

Consider evolution operator for a small time interval  $dt$

$$\psi(x, t + dt) = L[\psi(x, t)] = e^{dtiH}\psi(x, t) \quad (18)$$

$$\psi(x, t + dt) \approx (I + dtiH)\psi(x, t) = \psi(x, t) + dtiH\psi(x, t) \quad (19)$$

$$\frac{\psi(x, t + dt) - \psi(x, t)}{dt} \approx iH\psi(x, t) \quad (20)$$

In the limit  $dt \rightarrow 0$  we have obtained **non-stationary Schrödinger equation** for the evolution of  $\psi(x, t)$ :

$$\frac{\partial \psi(x, t)}{\partial t} = iH\psi(x, t)$$

this is also can be represented in the form

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H}\psi(x, t) \quad (21)$$

# Quantum mechanics formalism

There are two key objects in quantum mechanics: states and observables.

- ▶ **States** - vectors from a Hilbert space  $\mathcal{H}$ .  
They are denoted as  $|\psi\rangle$
- ▶ States are always latent, we can't observe them.
- ▶ **Observables** - Hermitian operators  $A : \mathcal{H} \rightarrow \mathcal{H}$ ,  $A^\dagger = A$ .
- ▶ Given a state  $|\psi\rangle$  can observe eigenvalues of operators in experiments. Since eigenvalues of Hermitian operators are real then we observe some real numbers.

# Quantum mechanics formalism

- Given a state  $|\psi\rangle$  can observe eigenvalues of operator  $A$  in experiments.

$$A|a\rangle = a|a\rangle \quad (22)$$

Probability to observe eigenvalue  $a$  equals to

$$\langle a|\psi\rangle = \int a(x, t)^* \psi(x, t) dx$$

**Spectral theorem.** Eigenvectors of any Hermitian  $A : \mathcal{H} \rightarrow \mathcal{H}$  operator form a complete basis of the Hilbert space  $\mathcal{H}$ .

$$I = \sum_{a \in \text{discrete spec}} |a\rangle\langle a| + \int_{\text{cont. spec}} |a\rangle\langle a| da = \sum_a |a\rangle\langle a| \quad (23)$$



# Quantum mechanics formalism

**Spectral theorem.** Eigenvectors of any Hermitian  $A : \mathcal{H} \rightarrow \mathcal{H}$  operator form a complete basis of the Hilbert space  $\mathcal{H}$ .

$$I = \sum_{a \in \text{discrete spec}} |a\rangle\langle a| + \int_{\text{cont. spec}} |a\rangle\langle a| da = \sum_a |a\rangle\langle a| \quad (24)$$

$$|a\rangle, |a\rangle \in \text{discrete spectrum} : \langle a|a'\rangle = \delta_{a,a'}$$

$$|a\rangle, |a\rangle \in \text{continuous spectrum} : \langle a|a'\rangle = \delta(a - a')$$

# Quantum mechanics formalism

## Examples of non-normalizable states

Consider an differential operator acting in the  $L_2$  Hilbert spaces of functions called momentum operator

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad (25)$$

By solving corresponding eigenvalue problem

$$\hat{p}\psi(x) = \frac{\hbar}{i} \frac{\partial \psi(x)}{\partial x} = p\psi(x), \quad (26)$$

where  $p$  is an eigenvalue, we get a solution for eigenfunctions

$$\psi_p(x) = Ce^{i\frac{px}{\hbar}} \quad (27)$$

Since the eigenvalue  $p$  can be arbitrary the momentum operator has continuous spectrum.

# Quantum mechanics formalism

## Examples of non-normalizable states

We get a solution for eigenfunctions of the momentum operator

$$\psi_p(x) = Ce^{i\frac{px}{\hbar}}$$

Consider normalization condition

$$\begin{aligned}\langle p'|p\rangle &= \int_{-\infty}^{\infty} dx (Ce^{i\frac{p'x}{\hbar}})^* \cdot Ce^{i\frac{px}{\hbar}} = \\ &= \int_{-\infty}^{\infty} dx C^* e^{-i\frac{p'x}{\hbar}} \cdot Ce^{i\frac{px}{\hbar}} = |C|^2 \int_{-\infty}^{\infty} dx e^{i\frac{x}{\hbar}(p'-p)} = \\ &= 2\pi\hbar\delta(p-p')\end{aligned}\tag{28}$$

Here we see that formally  $\langle p|p\rangle = \infty$  and we have to use normalization on the delta-function:  $\langle p'|p\rangle = \delta(p-p')$ . The constant  $C$  then equals to  $C = \frac{1}{\sqrt{2\pi\hbar}}$ .

# Quantum mechanics formalism

## Examples of non-normalizable states

**Problem:** non-normalizable states, for example eigenfunctions of the momentum operator

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}}$$

have infinite  $L_2$  norm and therefore don't lie in the Hilbert space of  $L_2$  integrable functions. **Does it make sense to consider such functions at all?**

**Solution:** we should extend our notion of Hilbert space  $\rightarrow$  Rigged Hilbert space.

Operator considered in quantum mechanics act on a Rigged Hilbert space (the space is also known as Gelfand triple, nested Hilbert space, or equipped Hilbert space).

More about the Rigged Hilbert spaces:

<http://galaxy.cs.lamar.edu/~rafaelm/webdis.pdf>

# Quantum mechanics formalism

Analogy with classical probability theory

- ▶  $\rho(x, t)$  - state = probability distributions;
- ▶  $f(x), x \sim \rho(x, t)$  - observables = values of some functions  $f(x)$  at samples
- ▶ Classical averages  $\langle f \rangle = \int f(x) \rho(x, t) dx$
- ▶ Quantum averages  $\langle f \rangle = \langle \psi | F | \psi \rangle = \int \psi(x, t)^* F \psi(x, t) dx$

# References

## **General introduction to quantum mechanics**

- ▶ Sakurai, J. J., and J. Napolitano. "Modern Quantum mechanics, 2: nd edition." Person New International edition (2011). <https://kgut.ac.ir/useruploads/1505647831850hcd.pdf>

## **Relations between Schrödinger equation, stochastic processes and optimal transport**

- ▶ Nelson, Edward. "Derivation of the Schrödinger equation from Newtonian mechanics." Physical review 150.4 (1966): 1079.
- ▶ Chow, Shui-Nee, Wuchen Li, and Haomin Zhou. "A discrete Schrödinger equation via optimal transport on graphs." Journal of Functional Analysis 276.8 (2019): 2440-2469.

# References

## **Rigged Hilbert spaces**

- ▶ De la Madrid, Rafael. "The role of the rigged Hilbert space in quantum mechanics." European journal of physics 26.2 (2005): 287.

## **On the representation theory of Lie groups in Rigged Hilbert Spaces**

- ▶ Celeghini, Enrico, Manuel Gadella, and Mariano A. del Olmo. "Groups, special functions and rigged Hilbert spaces." Axioms 8.3 (2019): 89.