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

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

We know that for all t out probability distribution is normalized

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

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Could we interpret this normalization condition

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

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

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

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 $\rho(x,t)$

$$\sqrt{\rho(x,t)} \to \sqrt{\rho(x,t)}e^{iS(x,t)} \tag{5}$$

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Then the normalization condition

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

becomes

$$||\sqrt{\rho(x,t)}e^{iS(x,t)}||_{L_2} = \int \left(\sqrt{\rho(x,t)}e^{iS(x,t)}\right)^* \sqrt{\rho(x,t)}e^{iS(x,t)}dx =$$

$$= \int \sqrt{\rho(x,t)}e^{-iS(x,t)}\sqrt{\rho(x,t)}e^{iS(x,t)}dx =$$

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

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

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

Informal Introduction

Note about Hilbert spaces:

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

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

- inner product $\to$ 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

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

What can we say about the evolution equation

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

in terms of $\psi(x,t)$?
Assume that evolution is described by an action of some operator $L : \mathcal{H} \to \mathcal{H}$ on the Hilbert space $\mathcal{H}$

$$\psi(x,t') = L[\psi(x,t)] \tag{10}$$

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 $\mathcal{H}$

$$\psi(x, t') = L[\psi(x, t)] \tag{11}$$

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.

$$\psi(x, t') = L[\psi(x, t)] \tag{12}$$

- 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

$$L = e^{g} \tag{13}$$

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 ∞-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: $\{$group$\} \to \{$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 ∞-dimensional representation consists of elements of the form $a\frac{d}{dx}, \quad a \in \mathbb{R}$.

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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

$$L_{t,t} = I \tag{14}$$

and that

$$L_{t,t'} \cdot L_{t',t''} = L_{t,t''} \tag{15}$$

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

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

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

Informal Introduction

From the point of view of Lie algebra

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

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

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

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

$$\psi(x, t + dt) \approx (I + dtiH)\psi(x, t) = \psi(x, t) + dtiH\psi(x, t) \tag{19}$$

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

In the limit $dt \to 0$ 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

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

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 $A : \mathcal{H} \to \mathcal{H}, \quad A^\dagger = A$.
- 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.

$$A|a\rangle = a|a\rangle \tag{22}$$

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 $A : \mathcal{H} \to \mathcal{H}$ operator form a complete basis of the Hilbert space $\mathcal{H}$.

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

Quantum mechanics formalism

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

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

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

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

Quantum mechanics formalism

Examples of non-normalizable states

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

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{25}$$

By solving corresponding eigenvalue problem

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

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

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

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

$$\langle p'|p\rangle = \int_{-\infty}^{\infty} dx (Ce^{i\frac{p'x}{\hbar}})^* \cdot Ce^{i\frac{px}{\hbar}} = \tag{28}$$

$$= \int_{-\infty}^{\infty} dx C^* e^{-i\frac{p'x}{\hbar}} \cdot Ce^{i\frac{px}{\hbar}} = |C|^2 \int_{-\infty}^{\infty} dx e^{\frac{ix}{\hbar}(p'-p)} =$$

$$= 2\pi\hbar\delta(p-p')$$

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

Additional material: Nelson's stochastic mechanics

There are more deep connections between quantum mechanics and classical probability theory / theory of stochastic processes. These analogies could be illustrated via so-called Nelson's approach to quantum mechanics.

Nelson assumed that trajectories $x(t)$ of quantum particles could be described using a stochastic differential Langevin equation. The Schrödinger equation could be derived form the Fokker-Planck equation on probability density $\rho(x(t))$.

Recall the Schrödinger equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t) = \left[-\frac{\hbar}{2}\Delta + V(x)\right]\psi(x,t) \qquad (29)$$

and represent the wave function as

$$\psi(x,t) = e^{\frac{1}{\hbar}(R(x,t)+iS(x,t))} \qquad (30)$$

Additional material: Nelson's stochastic mechanics

For the representation

$$\psi(x,t) = e^{\frac{1}{\hbar}(R(x,t)+iS(x,t))} \tag{31}$$

probability density becomes

$$\rho(x,t) = \psi(x,t)^*\psi(x,t) = e^{\frac{1}{\hbar}(R(x,t)-iS(x,t))}e^{\frac{1}{\hbar}(R(x,t)+iS(x,t))} \tag{32}$$

or

$$\rho(x,t) = e^{\frac{2}{\hbar}R(x,t)}. \tag{33}$$

In other words, the function $R(x,t)$ represents the log-likelihood

$$R(x,t) = \frac{\hbar}{2}\log\rho(x,t) = \hbar\log\sqrt{\rho(x,t)} \tag{34}$$

Additional material: Nelson's quantum mechanics

We have a representation

$$\psi(x,t) = e^{\frac{1}{\hbar}(R(x,t)+iS(x,t))} \tag{35}$$

From the Schrödinger equation for $\psi(x,t)$ we could obtain a system of PDEs for $R(x,t)$ and $S(x,t)$ called the stochastic Hamilton-Jacobi equations:

$$\frac{\partial R}{\partial t} + \nabla_i R \nabla^i S + \frac{\hbar}{2}\Delta S = 0 \tag{36}$$

$$\frac{\partial S}{\partial t} + \frac{1}{2}\left(\nabla_i S \nabla^i S - \nabla_i R \nabla^i R\right) + V - \frac{\hbar}{2}\Delta R = 0 \tag{37}$$

These equations could be seen as a generalization of the Hamilton-Jacobi equations from classical mechanics.

Additional material: Hamilton-Jacobi formalism

Classical mechanics systems are described by a Hamiltonian $H(p, q)$ which depends on the coordinates q and momentum p. The main idea of Hamilton-Jacobi approach is to find a change of variables

$$Q = Q(p, q)$$

$$P = P(q, p)$$

such that in new coordinates P, Q the Hamiltonian $H'(P, Q) \equiv 0$ equals to zero and the Hamiltianial equations reduce to the conservation laws:

$$\frac{dP(t)}{dt} = \frac{\partial H'(Q, P)}{\partial Q} = 0 \tag{38}$$

$$\frac{dQ(t)}{dt} = -\frac{\partial H'(Q, P)}{\partial P} = 0 \tag{39}$$

Additional material: Hamilton-Jacobi formalism

How to find such a change of variables (called canonical transformations or symplectomorphisms)?
Canonical transformations could be described by a generating function $S(q, Q, t)$:

$$P_i dQ_i - H'(P, Q)dt = p_i dq_i - H(p, q)dt - dS(q, Q, t) \qquad (40)$$

From the above equation it follows that the new Hamiltonian $H'(P, Q)$ is related to the old Hamiltonian $H(p, q)$ as

$$H'(P, Q) = H(p(P, Q), q(P, Q)) + \frac{\partial S(q(P, Q), Q, t)}{\partial t} \qquad (41)$$

Since we want the new Hamiltonian to be equal to zero we obtain the Hamilton-Jacobi equation on the unknown generating function $S(q, Q, t)$

$$\frac{\partial S(q, Q, t)}{\partial t} + H\left(\frac{\partial S(q, Q, t)}{\partial q}, q\right) = 0 \qquad (42)$$

Additional material: Hamilton-Jacobi formalism

Classical Hamilton-Jacobi equation:

$$\frac{\partial S}{\partial t} + H\left(x, \frac{\partial S}{\partial x}\right) = 0 \tag{43}$$

and for Hamiltonian $H(x, u) = \frac{\hbar}{2}u^2 + V(x)$ we get

$$\frac{\partial S}{\partial t} + \frac{\hbar}{2}(\nabla S)^2 + V = 0 \tag{44}$$

which is particular case of the stochastic Hamilton-Jacobi equations when $\hbar \to 0$ and similarly $R = \frac{\hbar}{2} \log \rho(x, t) \to 0$.

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