Quantum Probability

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Facets of Probabilty, Jena, 01.04.2026

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Introduction

quantum theory ⇔ probability

- very close relation
- very large topic
- concentrate here on *some* specific questions
- some literature

  [Dénes Petz, *Quantum Information Theory and Quantum Statistics* (2008)]
  [Michael A. Nielsen, Isaac L. Chuang, *Quantum Computation and Quantum Information* (2011)]
  [Alexander S. Holevo, *Quantum Systems, Channels, Information* (2012)]
  [Masahito Hayashi, *Quantum Information Theory* (2017)]

Quantum mechanics

- quantum theory works with *non-commuting operators*
- example: position $\mathbf{x}$ and momentum $\mathbf{p} = -i\hbar\boldsymbol{\nabla}$

$$\left[x_j, p_k\right] = \left[x_i, -i\hbar\frac{\partial}{\partial x_k}\right] = i\hbar\delta_{jk}$$

- example: spin components $\hat{s}_j = \frac{\hbar}{2}\sigma_j$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- technically: hermitian or self-adjoint operators in a Hilbert space (here: L^2, $\mathbb{C}^2$)
- closely related: inevitable effect of measurement
- closely related: uncertainty relations

Density matrices as quantum probabilities

- hermitian matrix or self-adjoint operator in a Hilbert space

$$\rho_{ij} = \rho_{ji}^*, \qquad \rho = \rho^\dagger$$

- can be diagonalized through unitary matrix or operator U

$$U^\dagger \rho U = \begin{pmatrix} p_1 & 0 & 0 & \dots \\ 0 & p_2 & 0 & \dots \\ 0 & 0 & p_3 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

- non-negative eigenvalues $p_k \geq 0$
- can often be normalized like probability

$$\mathrm{Tr}\{\rho\} = \sum_k p_k = 1$$

Expectation values

- observables are self-adjoint operators A
- spectral decomposition with real eigenvalues a_j and projectors P_j, schematically

$$A = \sum_j a_j \mathrm{P}_j$$

- probability to find result a_j is

$$w_j = \mathrm{Tr}\{\rho \mathrm{P}_j\}$$

- expectation values

$$\langle A \rangle = \mathrm{Tr}\{\rho A\} = \sum_j w_j a_j$$

Pure states and mixed states

- pure state

$$\rho_{ij} = \psi_i \psi_j^* \qquad\qquad \rho = |\psi\rangle\langle\psi|$$

  only one non-vanishing eigenvalue $p = 1$
- mixed state

$$\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$$

  at least two non-vanishing eigenvalues $p_k > 0$
- complete projective measurement leads to pure state
- general case are mixed states

Finite and infinite dimensions

- real quantum systems have infinitely many dimensions
- only simple and reduced models are described by finite dimensional density matrices
- examples: photon polarization, electron spin, *n*-level system

Two-level quantum system

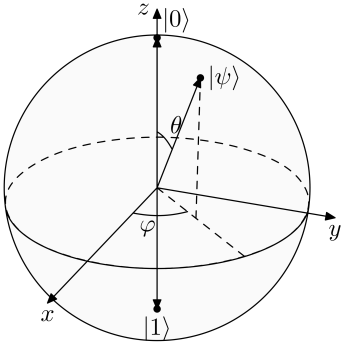
- *qubit*: Hilbert space $\mathbb{C}^2$
- basis $|0\rangle$ and $|1\rangle$
- density matrix, with $x^2 + y^2 + z^2 \leq 1$

$$\rho = \frac{1}{2}\begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix}$$

- Bloch sphere
- surface = pure states $\rho = |\psi\rangle\langle\psi|$

$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\varphi}\sin(\theta/2)|1\rangle$$

- interior = mixed states



Quantum correlation functions are not unique!

- several possible correlation function of *two* observables A, B
  - first choice
$$\mathrm{Tr}\{\rho AB\}$$
  - second choice
$$\mathrm{Tr}\{A\rho B\} = \mathrm{Tr}\{\rho BA\}$$
  - third choice
$$\mathrm{Tr}\{\sqrt{\rho}A\sqrt{\rho}B\}$$
  - Bogoliubov-Kubo-Mori
$$\int_0^1 d\lambda \mathrm{Tr}\{\rho^{1-\lambda}A\rho^{\lambda}B\}$$
- classical limit: A, B and ρ can be diagonalized simultaneously $\sum_j p_j a_j b_j$

Quantum evolution: isolated or open

- isolated quantum systems have unitary evolution

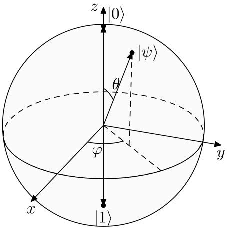
$$\rho \to U\rho U^\dagger \qquad U^\dagger U = \mathbb{1}$$

- open quantum systems evolve with completely positive, trace-preserving map

$$\rho \to \alpha(\rho) = \sum_n K_n \rho K_n^\dagger \qquad \sum_n K_n^\dagger K_n = \mathbb{1}$$

Distinguishing quantum states

- how well can quantum states be distinguished?
- which states should be considered close or far?
- is there a natural Riemannian metric for density matrices ρ_ξ?
  [Morozova, Chentsov (1990)]
- no unique metric on quantum states but one for every *operator monotone function* $f(z)$
  [Petz (1994)]



The ideas of information geometry

[Ronald A. Fisher, Calyampudi R. Rao, Shun'ich Amari, Nikolai N. Chentsov, ...]

- studies spaces of probability distributions $p_\xi(x)$ with parameters ξ^α
- Riemannian metric: Fisher information metric
- unique metric that is invariant under sufficient statistics [Chentsov (1972)]
- higher geometric structure: pair of dual connections and more [Amari, Chentsov, ...]
- geometric structure follows from a *divergence* or *relative entropy*
- useful also for statistical field theories [Floerchinger (2023), (2024)]

Classical probabilities, Fisher and Chentsov

- random variable x with probability distribution $p_\xi(x)$ where ξ^α are parameters
- map to new random variable $x \to y = f(x)$ with probability distribution $q_\xi(y)$

$$p_\xi(x) = p_\xi(x|y) q_\xi(y)$$

- *sufficient statistic*: no information about ξ is lost in the map
- technical condition: $p_\xi(x|y)$ independent of ξ
- Chentsov's theorem: unique invariant metric for sufficient statistic is Fisher metric

$$G_{\alpha\beta}(\xi) = \int dx \, p_\xi(x) \left(\frac{\partial}{\partial \xi^\alpha} \ln p_\xi(x) \right) \left(\frac{\partial}{\partial \xi^\beta} \ln p_\xi(x) \right)$$

- sufficient statistics: distance invariant
- non-sufficient statistics: distance decreases

Square roots of probabilities

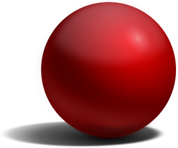
- Fisher information metric can be written as

$$G_{\alpha\beta}(\xi) = 4 \int dx \left(\frac{\partial}{\partial \xi^\alpha} \sqrt{p_\xi(x)} \right) \left(\frac{\partial}{\partial \xi^\beta} \sqrt{p_\xi(x)} \right)$$

- for discrete random variable take coordinates

$$p_j = \xi_j^2 \qquad\qquad j = 1, \ldots, N$$

- normalization $\xi_1^2 + \ldots + \xi_N^2 = 1$
- Fisher information metric induced Euclidean metric on the sphere!



Kullback-Leibler divergence on classical probabilties

- classical relative entropy or Kullback-Leibler divergence

$$D(p\|q) = \sum_j p_j \ln(p_j/q_j)$$

- not symmetric distance measure, but a *divergence*

$$D(p\|q) \geq 0 \qquad \text{and} \qquad D(p\|q) = 0 \quad \Leftrightarrow \quad p = q$$

- defines Fisher information metric for close-by distributions

$$D(p_\xi \| p_{\xi + d\xi}) = \frac{1}{2} G_{\alpha\beta}(\xi) d\xi^\alpha d\xi^\beta + \ldots$$

Significances of Kullback-Leibler divergence

Asymptotic frequencies

- true distribution q_j and frequency after N drawings $p_j = N(x_j)/N$
- probability to find frequencies p_j for large N
  (similar: Sanov's theorem, large deviation theory)

$$\sim \exp\left(-ND(p\|q)\right)$$

- probability for fluctuation around expectation value $\langle p_j \rangle = q_j$ tends to zero for large N and when divergence $D(p\|q)$ is large

Quantum relative entropy

[Umegaki (1962)]

- quantum relative entropy of two density matrices (also a *divergence*)

$$D(\rho\|\sigma) = \mathrm{Tr}\left\{\rho\left(\ln\rho - \ln\sigma\right)\right\}$$

- signals how well state ρ can be distinguished from a model σ
- Gibbs inequality: $D(\rho\|\sigma) \geq 0$
- $D(\rho\|\sigma) = 0 \quad \Leftrightarrow \quad \rho = \sigma$
- invariant under unitary dynamics for isolated systems

$$D(\rho\|\sigma) = D(U\rho U^\dagger\|U\sigma U^\dagger)$$

- but decreases in general for open quantum system dynamics

$$D(\rho\|\sigma) \geq D(\alpha(\rho)\|\alpha(\sigma))$$

Generalized relative entropies

[Petz (1988)]

- relative modular super operator Δ defined as

$$\Delta(A) = \sigma A \rho^{-1}$$

- self-adjoint with respect to Hilbert-Schmidt inner product
- functions $f(\Delta)$ are also well defined with $f(z)$ a function on $\mathbb{R}_+$
- generalized relative entropy (classical analog defined by [Csiszár (1967)])

$$D_f(\rho\|\sigma) = \text{Tr}\{\rho\, f(\Delta)\}$$

- decreases for open quantum system dynamics if $f(z)$ *operator monotone*

$$D_f(\rho\|\sigma) \geq D_f(\alpha(\rho)\|\alpha(\sigma))$$

Operator monotone functions

- hermitian matrix or operator A positive $A \geq 0$ means *all* eigenvalues $a_j \geq 0$
- *partial* order on hermitian matrices or operators

$$A \geq B \qquad \Leftrightarrow \qquad A - B \geq 0$$

- function $f(\Lambda)$ for diagonal matrix or operator Λ maps eigenvalues $\lambda_j \to f(\lambda_j)$
- for general hermitian matrix or self-adjoint operator $f(A) = f(U\Lambda U^\dagger) = Uf(\Lambda)U^\dagger$
- function $f(z)$ is *operator monotone* when

$$A \geq B \qquad \Rightarrow \qquad f(A) \geq f(B)$$

- depends on matrix dimension of A and B
- general characterization of operator monotone functions $f(z)$ by Loewner's theorem [Loewner (1934)]

General quantum correlation functions

[Petz (2002)]

- define superoperators $L_\rho A = \rho A$ and $R_\rho A = A\rho$
- define generalized correlation function

$$\Delta^f_{AB} = \text{Tr}\left\{A\, f\left(L_\rho R_\rho^{-1}\right) R_\rho B\right\}$$

- example $f(z) = z^\gamma$

$$\Delta^f_{AB} = \text{Tr}\left\{\rho^{(1-\gamma)} A \rho^\gamma B\right\}$$

- well defined for operator monotone function $f(z)$

Conservation versus loss of information

- unitary evolution for closed quantum systems: conserves quantum information
- different quantum states remain distinguishable
- non-unitary evolution in open quantum systems: quantum information can get lost
- different quantum states become less distinguishable
- thermalization: generic state approaches thermal equilibrium state
- second law of thermodynamics

Quantum fields

- information geometry in the Euclidean domain [Floerchinger (2024)]
- renormalization group flow [Floerchinger (2023)]
- entropic uncertainty relations for quantum fields [Floerchinger, Haas, Schroefl (2021)]
- relative entropy for local thermalization and fluid dynamics
  [Floerchinger, Haas (2020)] [Dowling, Floerchinger, Haas (2020)]

Outlook and conclusions

- information theory helps to better understand quantum dynamics
- adaptation to quantum *fields* currently being developed: light, matter, forces
- conservation versus loss of quantum information
- conceptual important but also technically
- technical applications
    - quantum communication
    - quantum computation
    - quantum metrology
- relation between different *effective* quantum field theories