Quantum Machine Learning Seminars

Week 2: Mathematical Methods of Quantum Computing

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Outline

1. Hilbert Space

Hilbert Space

Space Properties

- Building block: ψ is a ket vector $|\psi\rangle$ with a dual copy bra $|\psi\rangle^\dagger = \langle\psi|$. Classical quantities as x, p turned out to be disguised matrices $\hat{x}, \hat{p}$.
- Components: A vector can't exist alone, it needs a space and basis/bases to describe it.
- Randomness & Reality: Solutions of Schrödinger equation (energy eigenvalues) are exact and determined. But finding the instantaneous $|\psi\rangle$'s components would result generally in complex transition amplitudes associated with expected probabilities upon being squared, i.e. the outcome is random.

Heisenberg (left) with Bohr (right) in Copenhagen 1934. Source: Fermilab, U.S. Department of Energy

Hilbert Space

Space Properties

- Completeness: From the transition amplitudes and their relations with probabilities, the sum of the squared components of vector ψ must be 1.
- Wave collapse: Once a measurement (the differential equation) is applied, the wave will transform into one of its components while other components disappear such that the probability of finding the system in that component becomes 1.
- Commutativity & Uncertainty: associated dynamical variables x, p do NOT commute as Heisenberg showed: $\boxed{[\hat{x}, \hat{p}] = i\hbar\mathbb{1}} \Rightarrow \boxed{\Delta x \Delta p \geq \hbar/2}$.

https://en.wikipedia.org/wiki/Max_Born

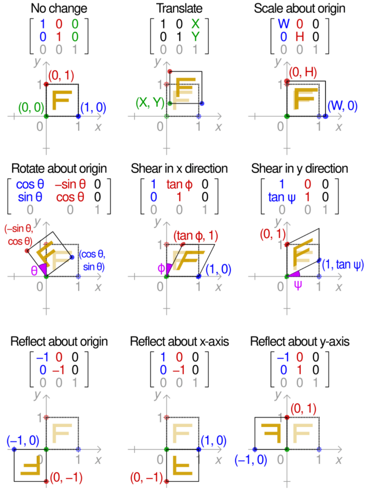
Inner Product Properties

- A finite-dimensional Hilbert space is the pair $(\mathtt{H}, \langle|\rangle)$ where $\mathtt{H} \equiv \mathbb{C}^n$ with inner product map $\langle|\rangle : \mathtt{H} \times \mathtt{H} \to \mathbb{C}$.
- $\langle\psi|\alpha\varphi + \beta\phi\rangle = \alpha\langle\psi|\varphi\rangle + \beta\langle\psi|\phi\rangle \;\; \forall \psi, \varphi, \phi \in \mathtt{H},\; \alpha, \beta \in \mathbb{C}$.
- $\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^* \quad \forall \psi, \varphi \in \mathtt{H}$.
- $\langle\psi|\psi\rangle > 0 \quad \forall \psi \neq 0,\; \psi \in \mathtt{H}$.
- $||\psi|| = \sqrt{\langle\psi|\psi\rangle}$,and $d(\psi, \varphi) := ||\psi - \varphi|| \; \forall \psi, \varphi \in \mathtt{H}$.
- $\forall \psi_i \in \mathtt{H} \equiv \mathbb{C}^n, \; \sum_{i=1}^{n} \alpha^i \psi_i = 0 \xLeftrightarrow{\{\phi_i\}_{i=1}^n} \alpha^i = 0 \; \forall \alpha^i \in \mathbb{C} \Rightarrow$
  $\psi = \sum_{i=1}^{m \leqslant n} \beta^i \psi_i \; \forall \psi \in \mathtt{H}$.
- $\{\phi_i^{\perp}\}_{i=1}^n \Leftrightarrow \langle\phi_i|\phi_j\rangle = \delta_{ij}$.

https://en.wikipedia.org/wiki/David_Hilbert

Linear Operators

- A linear operator A acting on the vectors of $\mathtt{H}$ is the map $A:\mathtt{H}\to\mathtt{H}$ with $A(\psi)\in\mathtt{H}\ \forall\psi\in\mathtt{H}$ such that $A(\alpha\psi+\beta\varphi)=\alpha A\psi+\beta A\varphi\ \forall\psi,\varphi\in\mathtt{H},\ \forall\alpha,\beta\in\mathbb{C}$, $(A+B)\psi=A\psi+B\psi$, and $A(\alpha\psi)=\alpha(A\psi)$.
- The set of linear operators on $\mathtt{H}$ is $\mathfrak{B}(\mathtt{H}):=\{A \text{ satisfying the above properties}\}$
- A is invertible if $\exists A^{-1}\in\mathfrak{B}(\mathtt{H})$ such that $AA^{-1}=A^{-1}A=\mathbb{1}$ and $\mathbb{1}\in\mathfrak{B}(\mathtt{H})$.
- For $\{\phi_i^{\perp}\}_{i=1}^{n}$, the linear trace of A is defined as $\mathrm{tr}(A):=\sum_{i=1}^{n}\langle\phi_i|A\phi_i\rangle\in\mathbb{C}$.
- $\mathrm{tr}(ABC)=\mathrm{tr}(BCA)=\mathrm{tr}(CAB)$.

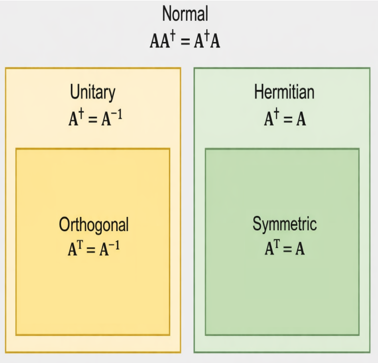


https://en.wikipedia.org/wiki/Transformation_matrix

Hilbert Space

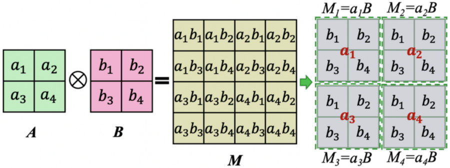
Eigenvalues and Spectral Theory

- The adjoint of operator $(A^T)^* = A^\dagger \in \mathfrak{B}(\mathtt{H})$ is unique for $A \in \mathfrak{B}(\mathtt{H})$ with $\langle A^\dagger \psi | \varphi \rangle = \langle \psi | A \varphi \rangle \ \ \forall \psi, \varphi \in \mathtt{H}$.
- A is self-adjoint (or Hermitian ?) if $A = A^\dagger$.
- The spectrum of A is the set of its eigenvalues: $\sigma(A) = \{\lambda \in \mathbb{C} : A\psi = \lambda\psi, \psi \in \mathtt{H} \backslash \{0\}\}$, and the eigenspace is $\mathtt{H}_\lambda = \{\psi, A\psi = \lambda\psi\} \subset \mathtt{H}$.
- Spectral theorem: For $A \in \mathfrak{B}(\mathtt{H})$, $A^\dagger A = AA^\dagger \Leftrightarrow \exists \{\phi_i^\perp\}_{i=1}^n, \ \phi_i^\perp \in \mathtt{H}_\lambda$.
- The eigenvalues of self-adjoint operator are real.
- For $U = (\phi_1^\perp, \phi_i^\perp, \cdots \phi_n^\perp)$ where $A\phi_i^\perp = A^\dagger \phi_i^\perp$, $D = UAU^\dagger$ with $D_{ii} = \lambda \in \sigma(A)$.



Tensor Product of Vectors

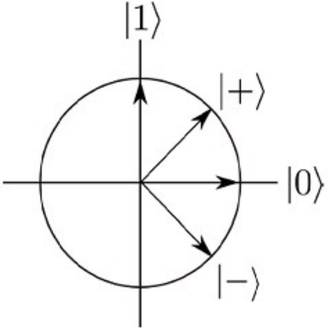
- For two different spaces $\mathtt{H}_A$ and $\mathtt{H}_B$ with $x, \psi \in \mathtt{H}_A$ and $y, \varphi \in \mathtt{H}_B$, the tensor product is the bilinear form:
  $\psi \otimes \varphi(x, y) = \langle \psi | x \rangle_A \langle \varphi | y \rangle_B.$
- The space $\mathtt{H}_A \otimes \mathtt{H}_B$ has inner product as
  $\langle \psi \otimes \varphi | \psi' \otimes \varphi' \rangle = \langle \psi | \psi' \rangle_A \langle \varphi | \varphi' \rangle_B$
  $\forall \psi, \psi' \in \mathtt{H}_A$ and $\varphi, \varphi' \in \mathtt{H}_B$.
- For $A \in \mathfrak{B}(\mathtt{H}_A)$ and $B \in \mathfrak{B}(\mathtt{H}_B)$, then
  $(A \otimes B)(\psi \otimes \varphi) = A\psi \otimes B\varphi.$
- $\mathfrak{B}(\mathtt{H}_A) \otimes \mathfrak{B}(\mathtt{H}_B) = \mathfrak{B}(\mathtt{H}_A \otimes \mathtt{H}_B)$, i.e., for $C \in \mathfrak{B}(\mathtt{H}_A \otimes \mathtt{H}_B)$, $C = \sum_k A_k \otimes B_k$.



Hilbert Space

Pure & Mixed States

- For $\{\phi_i\}_{i=1}^n$, the projector operator is
  $$P_\lambda = \sum_{i=1}^n |\phi_i\rangle \otimes \langle\phi_i| = \sum_{i=1}^n |\phi_i\rangle\langle\phi_i|.$$
- This means A can be decomposed into P_λ as
  $$A = \sum_{\lambda\in\sigma(A)} \lambda P_\lambda.$$
- Pure states are equivalence classes of unit vectors
  $|\psi\rangle \sim |\varphi\rangle \Leftrightarrow \exists\alpha \in \mathbb{R},\ |\psi\rangle = e^{i\alpha}|\varphi\rangle$ for $|\psi\rangle, |\varphi\rangle \in \mathtt{H}$
  and $\langle\psi|\psi\rangle = \langle\varphi|\varphi\rangle = 1$.
- For pure states, we define $A \equiv \rho_\psi := |\psi\rangle\langle\psi|$.
- For mixed states $\rho_\psi := \sum_i p_i|\psi_i\rangle\langle\psi_i|$ with $\sum_i p_i = 1,\ p_i \geqslant 0$.

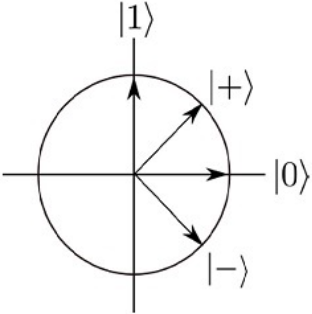


$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$
$$|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Hilbert Space

Coherent Superposition

- $\mathfrak{S}(\mathtt{H}) = \{\rho \in \mathfrak{B}(\mathtt{H}),\ \rho \geqslant 0,\ \operatorname{tr}(\rho) = 1\}$.
- Coherent Superposition $\Psi = \dfrac{\sum_i a_i|\psi_i\rangle}{||\sum_i a_i|\psi_i\rangle||} \in \mathtt{H},\ a_i \in \mathbb{C}$.
- $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \qquad \alpha, \beta \in \mathbb{C}, \qquad |\alpha|^2 + |\beta|^2 = 1.$
- $$\rho_{\text{coh}} = |\psi\rangle\langle\psi| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}.$$
- If two alternatives contribute amplitudes A_1 and A_2, then $P_{\text{coh}} = \left|A_1 + A_2\right|^2 = |A_1|^2 + |A_2|^2 + 2\operatorname{Re}(A_1^* A_2)$.
- For incoherent superposition, $\operatorname{Re}(A_1^* A_2) = 0$ and ρ_{incoh} is diagonal.



$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

Entanglement

- Pure states $|\psi\rangle \in \mathtt{H}_A$, $|\varphi\rangle \in \mathtt{H}_B$ define a composite pure state $|\psi\rangle \otimes |\varphi\rangle \in \mathtt{H}_A \otimes \mathtt{H}_B$, but a general $|\Psi\rangle$ need not factorize.
- A pure state is separable iff $|\Psi\rangle = |\psi\rangle \otimes |\varphi\rangle$; otherwise it is entangled; subsystems are correlated and no independent pure state description.
- A mixed state (density operator) ρ is separable iff $\rho = \sum_i p_i \, \rho_i^{(A)} \otimes \rho_i^{(B)}, \qquad p_i \geq 0, \quad \sum_i p_i = 1$; otherwise ρ is entangled.
- For pure states, the mixed-state separability condition reduces to the product-state criterion; e.g. $|\Psi\rangle = \frac{1}{\sqrt{2}}\big(|00\rangle + |11\rangle\big)$ is entangled and a local measurement on one qubit collapses the joint state (to $|00\rangle$ or $|11\rangle$).

Thank You!