

Methods in quantum computing

Mária Kieferová

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University of Technology Sydney

- Updated lecture notes from Lecture #1 and new notes for Lecture #2 are available
- Recording for Lecture #1 is available
- <https://jamboard.google.com/> is a useful tool for working on problems together
- Slack channel on SQA Slack for the class - let me know if you weren't added

Today

1. Linear algebra
2. Quantum states
3. Quantum operations
4. No-cloning theorem
5. Measurement

Linear algebra

$< \infty$
A d -dimensional Hilbert space \mathcal{H} is a vector space equipped with an inner product. Let $\{\mathbf{e}_i\}_{i=0}^{d-1}$ be the computational basis, where \mathbf{e}_i is a column vector of zeros except a '1' at the $(i+1)$ -th entry. Any vector $\mathbf{v} \in \mathcal{H}$ can be decomposed into basis vectors \mathbf{e}_i as

$$\mathbf{v} = \sum_{i=0}^{d-1} v_i \mathbf{e}_i = v_0 \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + v_1 \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \dots \quad (1)$$

for some complex number $v_i \in \mathbb{C}$. The inner product (or dot product) of two vectors \mathbf{u} and \mathbf{v} in the same basis in \mathcal{H} is defined as

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^\dagger \mathbf{v} = \sum_{i=0}^{d-1} u_i^* v_i, \quad (2)$$

where \dagger denotes transpose and conjugate.

$$\begin{pmatrix} | \\ \vdots \\ | \end{pmatrix} \rightarrow (a_0^* \ a_1^* \)$$

+ conjugate
+ transpose

Dirac notation

Denote $|i\rangle \equiv \mathbf{e}_i$ and write \mathbf{v} as $|v\rangle$:

$$|v\rangle = \sum_{i=0}^{d-1} v_i |i\rangle. \quad (3)$$

The inner product

$$\langle u|v\rangle = \sum_{i,j} u_i^* v_j \langle i|j\rangle = \sum_i u_i^* v_i \quad (4)$$

where $\langle u| \equiv |u\rangle^\dagger$ is now a row vector and $\langle i|j\rangle = \delta_{i,j}$.

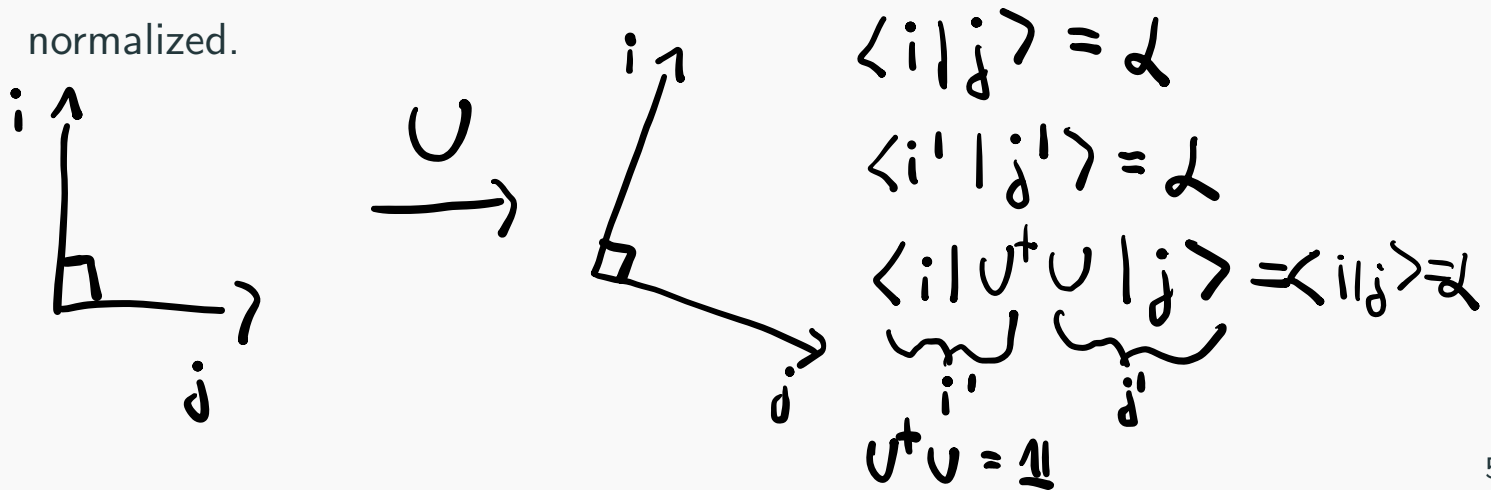
$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ \uparrow \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = 1$$

$$\begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Vector space basis

$\{|i\rangle\}$ set of mutually orthogonal normalized vectors.

For a unitary operator U , $\{U|i\rangle\}$ will be also mutually orthogonal and normalized.



Linear maps

$$L: U \rightarrow V$$

$$L(u_1) = v_1$$

$$L(u_2) = v_2$$

$$L(u_1 + \underset{\substack{\uparrow \\ \text{scalar}}}{d} u_2) = v_1 + d v_2$$

Example: Matrix multiplication

Linear operators

Given an linear operator L , there is an equivalent matrix representation

$[L_{i,k}]$ in the basis spanned by $\{|i\rangle\langle k|\}$:

$$L = \sum_{i,k=0}^{d-1} L_{i,k} |i\rangle\langle k|, \quad (5)$$

where $L_{i,k} = \langle i|L|k\rangle$. $L_{j,e} \langle j|L|e\rangle = \sum_{i,k} L_{i,k} \langle j|i\rangle \langle k|e\rangle = L_{j,e}$

An linear operator $H \in \mathcal{L}(\mathcal{H})$ is called Hermitian iff $H^\dagger = H$. For a Hermitian matrix H , the spectral theorem states that there exists an orthonormal basis $\{|\nu_i\rangle\}$ and real numbers $\{\lambda_i\} \in \mathbb{R}$ so that

$$H = \sum_i \lambda_i |\nu_i\rangle\langle \nu_i|. \quad (6)$$

Equivalently, $\{\lambda_i\}$ and $\{|\nu_i\rangle\}$ are known as eigenvalues and eigenvectors of H , respectively.

Exercise

Verify that Pauli X is a Hermitian operator and compute its eigenvalues and eigenvectors.

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Tensor product of Hilbert spaces

\mathcal{H}_A \mathcal{H}_B

Given two vectors $|u\rangle \in \mathcal{H}_A$ and $|v\rangle \in \mathcal{H}_B$, the tensor product ' \otimes ' of them is

$$|u\rangle \otimes |v\rangle = \sum_{i=0}^{d_A-1} \sum_{j=0}^{d_B-1} u_i v_j |ij\rangle, \quad (7)$$

a vector of $d_A d_B$ -dimension. If $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ are orthonormal bases in \mathcal{H}_A and \mathcal{H}_B , respectively, then $\{|i\rangle_A \otimes |j\rangle_B\}$, $i \in \{0, \dots, d_A - 1\}$ and $j \in \{0, \dots, d_B - 1\}$, forms an orthonormal basis in $\mathcal{H}_A \otimes \mathcal{H}_B$. The inner product on the space $\mathcal{H}_A \otimes \mathcal{H}_B$ is defined by

confusing notation!

$$(\langle u_1|_A \otimes \langle u_2|_B)(|v_1\rangle_A \otimes |v_2\rangle_B) = \langle u_1|v_1\rangle \langle u_2|v_2\rangle. \quad (8)$$

Tensor product for operators

Linear operators in $\mathcal{L}(\mathcal{H})$:

$$\begin{aligned} L \otimes M &= \left(\sum_{i,j=0}^{d_A-1} L_{i,j} |i\rangle\langle j| \right) \otimes \left(\sum_{k,\ell=0}^{d_B-1} M_{k,\ell} |k\rangle\langle \ell| \right) \\ &= \sum_{i,j=0}^{d_A-1} \sum_{k,\ell=0}^{d_B-1} L_{i,j} M_{k,\ell} \underbrace{|i\rangle\langle j| \otimes |k\rangle\langle \ell|}_{\text{new basis}}. \end{aligned} \quad (9)$$

? $\langle i | \otimes | j \rangle$

Trace

$$\text{Tr } L = \left(\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right)$$

The trace maps is defined as

$$\delta_{j \neq k} \left(\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right)$$

$$\text{Tr } |j\rangle\langle k| = \langle k|j\rangle = \delta_{k,j} \left(\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right) \quad (10)$$

From linearity, the trace of an operator L is

$$\text{Tr } L = \sum_{i=0}^{d-1} \langle i|L|i\rangle = \sum_j L_{j,j} \quad (11)$$

Exercise

- Cyclic property: Show that $\text{Tr } LM = \text{Tr } ML$.

$$\mathbb{1} = \sum_j |j\rangle\langle j|$$

- Show that $\text{Tr } A$ is independent of the basis of A .

$$\begin{aligned} \text{Tr}(LM) &= \sum_i \langle i | L M | i \rangle = \sum_{ij} \langle i | L | j \rangle \langle j | M | i \rangle \\ &= \sum_{ij} \langle j | M | i \rangle \langle i | L | j \rangle \\ &= \sum_j \langle j | M L | j \rangle = \text{Tr}(ML) \end{aligned}$$

product $M_{ij} L_{jk}$

$\text{Tr}(A) = \sum_i A_{ii}$

$\text{Tr}(ML) = \sum_i M_{ij} L_{ji}$

$\text{Tr}(LM)$

$$A = \sum_{ij} A_{ij} |i\rangle\langle j|$$

$|i\rangle \rightarrow U|i\rangle$

Partial trace



A generalization of a trace. Partial trace maps an operator to a lower-dimensional operator. Formally, partial trace

$\text{Tr}_A : \mathcal{L}(\mathcal{H}_{AB}) \rightarrow \mathcal{L}(\mathcal{H}_B)$ is defined by

$$\text{Tr}_A(|i\rangle\langle j|_A \otimes |k\rangle\langle l|_B) = \langle j|i\rangle |k\rangle\langle l|_B = \delta_{i,j} |k\rangle\langle l|_B. \quad (12)$$

For a composite system on the space $\mathcal{H}_A \otimes \mathcal{H}_B$, Tr_A gives trace only over the subsystem on \mathcal{H}_A and remains subsystem \mathcal{H}_B intact. We often say that we "trace-over A ".

Tr_B

Quantum states

Use the ket notation $|\cdot\rangle$ to denote a column vector of length one, e.g.,

$$|\psi\rangle := \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (13)$$

and use the bra notation $\langle\cdot|$ to denote the hermitian conjugate of $|\cdot\rangle$:

$$\langle\psi| := \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix}. \quad (14)$$

An alternative representation of a quantum state is the density matrix.

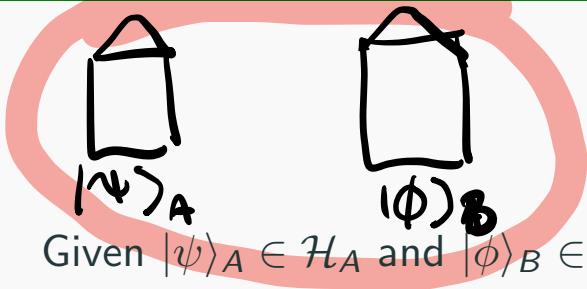
For pure states:

$$\left\{ |\psi\rangle, |\psi^\perp\rangle \right\} \leftarrow \sigma_\psi = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (15)$$

this basis

$\sigma_\psi = |\psi\rangle\langle\psi|$

Joint quantum state



Given $|\psi\rangle_A \in \mathcal{H}_A$ and $|\phi\rangle_B \in \mathcal{H}_B$, the joint quantum state is

$$|\varphi\rangle_{AB} \equiv |\psi\rangle_A \otimes |\phi\rangle_B \in \mathcal{H} \equiv \mathcal{H}_A \otimes \mathcal{H}_B.$$

If one of the subsystems, say \mathcal{H}_A , is lost from $|\varphi\rangle_{AB}$, the residue quantum state can be expressed as

$$|\phi\rangle\langle\phi|_B = \text{Tr}_A |\varphi\rangle\langle\varphi|. \quad (16)$$

$|\varphi\rangle$ is a general pure state $\text{Tr}_B |\varphi\rangle\langle\varphi| = |\psi\rangle\langle\psi|_A$
 $|\phi\rangle\langle\phi|_B$ might not have to be pure

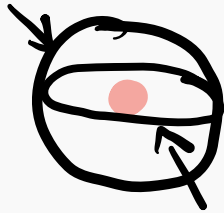
Exercise

$$\text{Tr}_A(|\Phi\rangle\langle\Phi|_{AB}) = \sigma_B \in \mathcal{R}_B$$

\uparrow
 $\mathcal{R}_A \otimes \mathcal{R}_B$

Let $|\Phi\rangle_{AB} = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B)$. Compute $\text{Tr}_A(|\Phi\rangle\langle\Phi|_{AB})$ and $\text{Tr}_B(|\Phi\rangle\langle\Phi|_{AB})$. Discuss whether the result could be a pure state (no need to prove it).

$\frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$ maximally mixed state
pure states → not pure



inside
are mixed states

Mixed states

Not pure states:

- outcome of a random preparation
- part of a larger entangled state

An ensemble of pure states $\mathcal{E} : \{p_i, |\psi_i\rangle\}$ can be denoted by a density operator

$$\sigma := \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad \begin{array}{l} \text{before} \\ 0.5 \quad |0\rangle\langle 0| \\ 0.5 \quad |1\rangle\langle 1| \end{array} \quad (17)$$

where $|\psi_i\rangle$ are individual states that could be prepared and p_i are the corresponding probabilities. We refer to objects σ as **density matrices**.

Exercise

There are three necessary and sufficient criteria that a matrix corresponds to a valid description to a quantum state. Show that

probabilities
 $p_i \in [0, 1]$

$$\sigma := \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{18}$$

↑ projectors

where $\sum_i p_i = 1$ satisfies all three of them



1. σ is Hermitian ¹

2. σ is positive semi-definite ²

3. $\text{Tr}[\sigma] = 1$.

$$\sigma = \begin{pmatrix} p_0 & & & \\ & p_1 & & \\ & & \ddots & \\ & & & p_n \\ \hline & & & & 0 \end{pmatrix}$$

basis of $\{|\psi_i\rangle\}$

¹A hermitian matrix A satisfies $A^\dagger = A$.

²Eigenvalues of a positive semi-definitive matrix are real and equal to 0 or positive.

Pure states

If ρ is pure, it can be written as a projector on the corresponding pure state $|\psi\rangle$

$$\sigma_\psi = |\psi\rangle\langle\psi|. \quad (19)$$

$$\rho = \begin{pmatrix} \cdot & & & 0 \\ & \cdot & & \\ & & \cdot & \\ 0 & & & \cdot \end{pmatrix}$$

$$\rho^2 = \begin{pmatrix} a_{00}^2 & & & \\ & a_{11}^2 & & \\ & & \cdot & \\ & & & \cdot \end{pmatrix}$$

$$\rho_{\text{pure}} = \begin{pmatrix} 1 & & & 0 \\ & 0 & & \\ & & \cdot & \\ 0 & & & \cdot \end{pmatrix}$$

$$\rho_{\text{pure}}^2 = \begin{pmatrix} 1 & & & 0 \\ & 0 & & \\ & & \cdot & \\ & & & \cdot \end{pmatrix}$$

Church of the larger Hilbert space

Suppose that the person, say Alice, who prepares this ensemble can keep track of 'which state' she prepared. In other words, she has the additional classical label $|x\rangle\langle x|$ attached to the state $\sigma_x \in \mathcal{D}(\mathcal{H}_B)$, where $\{|x\rangle\}$ forms an orthonormal basis of \mathcal{H}_X . Such a hybrid classical-quantum system can be described as

$$\sigma_{XB} = \sum_{x \in \mathcal{X}} p_x |x\rangle\langle x| \otimes |\psi_x\rangle\langle \psi_x|. \quad (20)$$

Unitary evolution

$$|\psi\rangle \rightarrow U|\psi\rangle. \quad (21)$$

For a general quantum state described by a density matrix (21) takes form

$$\rho \rightarrow U\rho U^\dagger = \sum_i U|\psi_i\rangle\langle\psi_i|U^\dagger. \quad (22)$$

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$|\psi_i\rangle \rightarrow U|\psi_i\rangle$$

$$\rho \rightarrow \sum_i p_i U_i |\psi_i\rangle\langle\psi_i| U_i^\dagger$$

Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle \quad \hbar = 1 \quad \rightarrow \text{Hermitian} \quad (23)$$

where \hbar is the Planck constant and H is the system Hamiltonian.

Eigenvalues of Hamiltonian define the allowed energies of a system.

Physicists and chemists really care about this!!

$$\begin{array}{l} \nearrow \\ 2^n \text{ vector} \end{array} |\psi(t)\rangle = \underbrace{e^{-iHt}}_{\text{unitary operation}} |\psi(0)\rangle \quad \leftarrow 2^n \times 2^n \text{ matrix}$$

Exercise

Define purity of a quantum state as $\text{Tr}[\rho^2]$. Show that unitary operations preserve purity, i.e. a pure state never gets mapped onto a mixed state and vice versa.

pure $\text{Tr}(\rho^2) = 1$

mixed $\text{Tr}(\rho^2) < 1$

$$\rho \rightarrow U \rho U^\dagger$$

$$\text{Tr}(U \rho U^\dagger U \rho U^\dagger)$$

$$= \text{Tr}(U \rho \rho U^\dagger)$$

END OF
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Channels are the most general operation of quantum states. They must be always map quantum states onto quantum states, even if we apply the channel only on a subset of qubits. Any such channel can be written as

$$\Phi(\sigma) = \sum_i B_i \sigma B_i^\dagger \quad \text{where} \quad \sum_i B_i B_i^\dagger = 1. \quad (24)$$

No cloning theorem

Theorem (No-Cloning theorem)

There is no unitary operation U_{copy} on $\mathcal{H}_A \otimes \mathcal{H}_B$ such that for all

$|\psi\rangle_A \in \mathcal{H}_A$ and $|0\rangle_B \in \mathcal{H}_B$

$$U_{\text{copy}}(|\phi\rangle_A \otimes |0\rangle_B) = e^{if(\phi)}|\phi\rangle_A \otimes |\phi\rangle_B \quad (25)$$

for some number $f(\phi)$ that depends on the initial state $|\phi\rangle$.

Exercise

Prove the no-cloning theorem by contradiction.

- a Assuming U_{copy} exists, take two states $|\phi_A\rangle$ and $|\psi\rangle$. Now apply U_{copy} on both of them and compute the resulting inner product $(\langle\phi|_A \otimes \langle 0|_B)U_{\text{copy}}^\dagger U_{\text{copy}}(|\psi\rangle_A \otimes |0\rangle_B)$.
- b Explain how (a) leads to a contradiction.

Quantum measurement

Obtain classical information from a quantum state. It can destroy the superposition property of a quantum state.

Observe this qubit in state $|0\rangle$ with probability $|\alpha|^2$ and in state $|1\rangle$ with probability $|\beta|^2$. Furthermore, after the measurement, the qubit state $|b\rangle$ will disappear and collapse to the observed state $|0\rangle$ or $|1\rangle$.



General quantum measurement

A collection of $\Upsilon := \{M_i\}$, where each measurement operator $M_i \in \mathcal{L}(\mathcal{H})$ satisfies

$$\sum_i M_i = I \quad (26)$$

and each M_i is positive semi-definite operator. We call this measurements positive operator-valued measure (POVM). The probability of obtaining an outcome i on a quantum state ρ is

$$p_i := \text{Tr}(M_i \rho). \quad (27)$$

The state after measurement will be altered as

$$\rho_i := \frac{M_i \rho}{p_i}.$$

Projective measurement

Each M_i is a projector

$$p_j := \text{Tr}(P_j|\phi\rangle\langle\phi|)$$

and the resulting state

$$\frac{P_j|\phi\rangle}{\sqrt{p_j}}.$$