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- Distance measures of density matrices: fidelity & trace distance
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Learning goals:

Distance measures for quantum states:

Two common distance measures for states ρ, σ are

Trace distance: $D(\rho, \sigma) = \frac{1}{2} \text{Tr} |\rho - \sigma|$

Here $|A| = \sqrt{A^\dagger A}$ is a positive operator.

For hermitian $A = A^\dagger$, $\text{Tr} |A| = \sum_i |\lambda_i|$, where λ_i are the (real) eigenvalues of A .

Example:

① If $[\rho, \sigma] = 0 \Rightarrow$ can be diagonalized in the

same basis $\rho = \sum_i p_i |i\rangle\langle i|$, $\sigma = \sum_i s_i |i\rangle\langle i|$

$$\begin{aligned} \Rightarrow D(\rho, \sigma) &= \frac{1}{2} \text{Tr} \left| \sum_i (p_i - s_i) |i\rangle\langle i| \right| = \\ &= \frac{1}{2} \text{Tr} \sqrt{\sum_{i,j} (p_i - s_i)(p_j - s_j) |j\rangle\langle j| |i\rangle\langle i|} = \\ &= \frac{1}{2} \text{Tr} \sqrt{\sum_i (p_i - s_i)^2 |i\rangle\langle i|} = \\ &= \frac{1}{2} \text{Tr} \left[\sum_i |p_i - s_i| |i\rangle\langle i| \right] = \end{aligned}$$

$$\Leftrightarrow D(\rho, \sigma) = \frac{1}{2} \sum_i |\rho_i - \sigma_i| \text{ if } [\rho, \sigma] = 0.$$

This turns out to be the definition of the L_1 distance or Kolmogorov distance of classical probability distributions $\{\rho_i\}_{i \in X}$, $\{\sigma_i\}_{i \in X}$. ^{alphabet X}

$$\textcircled{2} \quad \rho = \frac{3}{4} |0\rangle\langle 0| + \frac{1}{4} |1\rangle\langle 1| = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}$$

$$\sigma = \frac{2}{3} |0\rangle\langle 0| + \frac{1}{3} |1\rangle\langle 1| = \begin{pmatrix} 2/3 & 0 \\ 0 & 1/3 \end{pmatrix}$$

$$\Rightarrow D(\rho, \sigma) = \frac{1}{2} \text{Tr} \sqrt{(\rho - \sigma)(\rho - \sigma)}$$

Now: $\rho - \sigma = \begin{pmatrix} 1/12 & 0 \\ 0 & -1/12 \end{pmatrix}$

$$\Rightarrow (\rho - \sigma)(\rho - \sigma) = \begin{pmatrix} 1/144 & 0 \\ 0 & 1/144 \end{pmatrix}$$

$$\Rightarrow \sqrt{(\rho - \sigma)(\rho - \sigma)} = \begin{pmatrix} 1/12 & 0 \\ 0 & 1/12 \end{pmatrix}$$

$$\Rightarrow D(\rho, \sigma) = \frac{1}{2} \cdot 2 \cdot \frac{1}{12} = \frac{1}{12}.$$

③ Trace distance between two single qubit states (HW).

Important properties (for proofs, see NDC):

- $D(U\rho U^\dagger, U\sigma U^\dagger) = D(\rho, \sigma)$ for unitary U

- $D(\rho, \sigma) = \max_{\{E_m\}} D(p_m, q_m)$

Here, $\{E_m\}$ denotes a POVM and $p_m = \text{Tr}(\rho E_m)$,

$$q_m = \text{Tr}(\sigma E_m).$$

Trace distance is upper bound on trace distance of classical probability distributions arising from measurements.

Or Tr distance is distance between the probability distributions achieved by the optimal measurement (optimal choice of POVM) for distinguishing the states.

- Strongly concave

distance b/w classical
probability distributions

$$D\left(\sum_i p_i \rho_i, \sum_i q_i \sigma_i\right) \leq D(p_i, q_i) + \sum_i p_i D(\rho_i, \sigma_i)$$

Fidelity:

$$F(\rho, \sigma) = \text{Tr} \sqrt{\rho^{1/2} \sigma \rho^{1/2}} = \text{Tr} |\sigma^{1/2} \rho^{1/2}|.$$

(sometimes also defined as $(\text{Tr} \sqrt{\rho^{1/2} \sigma \rho^{1/2}})^2$, e.g., in Preskill).

• $F(\rho, \sigma) = F(\sigma, \rho)$

• If $[\rho, \sigma] = 0 \Rightarrow F(\rho, \sigma) = \sum_i \sqrt{\rho_i \sigma_i} \equiv F(\rho_i, \sigma_i)$
fidelity of classical probability distributions

• $F(|\psi\rangle\langle\psi|, \rho) = \sqrt{\langle\psi|\rho|\psi\rangle}$

Overlap of pure state $|\psi\rangle$ and state ρ .

$\Rightarrow F = 1$ if states are identical

$F = 0$ if states are orthogonal

• F is not a metric, but we can use it to define one.

$A(\rho, \sigma) = \arccos F(\rho, \sigma)$ is a metric

Example:

$$\rho = \frac{3}{4} |0\rangle\langle 0| + \frac{1}{4} |1\rangle\langle 1| = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}$$

$$\sigma = \frac{2}{3} |0\rangle\langle 0| + \frac{1}{3} |1\rangle\langle 1| = \begin{pmatrix} 2/3 & 0 \\ 0 & 1/3 \end{pmatrix}$$

$$\begin{aligned} \Rightarrow F(\rho, \sigma) &= \text{Tr} \sqrt{\rho^{1/2} \sigma \rho^{1/2}} = \\ &= \text{Tr} \sqrt{\begin{pmatrix} \sqrt{3}/2 & \\ & 1/2 \end{pmatrix} \begin{pmatrix} 2/3 & \\ & 1/3 \end{pmatrix} \begin{pmatrix} \sqrt{3}/2 & \\ & 1/2 \end{pmatrix}} = \\ &= \text{Tr} \sqrt{\begin{pmatrix} 1/2 & \\ & 1/12 \end{pmatrix}} = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{12}} \approx 0.9958. \end{aligned}$$

Uhlmann's theorem (for proof, see N&C (pp. 410) or P.Ch. 2):

Let $\rho, \sigma \in \mathcal{H}_A$ be two quantum states. Introduce \mathcal{H}_R , which is a copy of \mathcal{H}_A :

$$F(\rho, \sigma) = \max_{|\psi\rangle, |\varphi\rangle} |\langle \psi | \varphi \rangle|,$$

where $|\psi\rangle$ is a purification of ρ and $|\varphi\rangle$ of σ on the extended space $\mathcal{H}_A \otimes \mathcal{H}_R$.

Fidelity of two density operators ρ, σ is the maximal possible overlap of their purifications.

• Strong concavity of fidelity:

$$F\left(\sum_i p_i \rho_i, \sum_i q_i \sigma_i\right) \geq \sum_i \sqrt{p_i q_i} F(\rho_i, \sigma_i).$$

Relation between trace distance $D(\rho, \sigma)$ & fidelity $F(\rho, \sigma)$:

Equivalent for pure states:

$$D(|a\rangle, |b\rangle) = \sqrt{1 - F(|a\rangle, |b\rangle)}.$$

Generally: ρ and σ are close in Tr distance iff their fidelity is close to one.

$$1 - F(\rho, \sigma) \leq D(\rho, \sigma) \leq \sqrt{1 - F(\rho, \sigma)^2}.$$

Our example (2) above: $D(\rho, \sigma) = \frac{1}{12}$, $F(\rho, \sigma) = \frac{1}{2} + \frac{1}{2\sqrt{3}}$.

$$\Rightarrow 1 - F = 4.2 \cdot 10^{-3} \leq \frac{1}{12} = 0.083 \leq \sqrt{1 - F^2} = 0.091.$$

Quantum channels:

What is the most general evolution of system A?

We learned two special cases: $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ with $|\psi_i\rangle \in H_A \equiv A$.

(i) unitary evolution $\rho \mapsto U \rho U^\dagger$

(ii) generalized measurement $\rho \mapsto \frac{M_a \rho M_a^\dagger}{\text{Tr}(M_a^\dagger M_a \rho)}$
 $= p(a)$

→ we learned that case (ii) corresponds to unitary evolution on an extended system followed by a projective measurement.

Unitary evolution (or isometry to be precise):

$$U : |\psi\rangle_A \otimes |0\rangle_E \mapsto \sum_a M_a |\psi\rangle \otimes |a\rangle_E$$

$$\text{on DM} \Rightarrow U : \rho = |\psi\rangle_A \langle\psi| \otimes |0\rangle_E \langle 0|_E \mapsto \sum_{a, a'} M_a |\psi\rangle \langle a|_E \langle\psi| \langle a'|_E M_{a'}^\dagger$$

$$\text{By convex linearity: } U : \rho = \rho_A \otimes |0\rangle_E \langle 0|_E \mapsto \sum_{a, a'} M_a \rho M_{a'}^\dagger \otimes |a\rangle_E \langle a'|_E$$

Projective measurement:

$$p(a) = \text{Tr} \left[\left(\mathbb{I}_A \otimes |a\rangle_E \langle a|_E \right) \sum_{a', a''} M_{a'} |\psi\rangle \langle a'|_E \langle\psi| \langle a''|_E M_{a''}^\dagger \right]$$

acts only on A

$$= \langle\psi| M_a^\dagger M_a |\psi\rangle$$

$$\text{By convex linearity: } p(a) = \text{Tr}(M_a^\dagger M_a \rho)$$

In the general case we may not observe the environment E or fail to record some or all of the projective measurement

outcomes. Then, we need to average over the possible post measurement states $\left\{ \rho_a = \frac{M_a \rho M_a^\dagger}{p(a)} \right\}$, weighted

with their respective probabilities $p(a) = \text{Tr}(M_a^\dagger M_a \rho)$.

Let us first consider the case when we fail to record any measurement outcome, i.e., trace out E .

$$\text{Then, } \sum_a M_a^\dagger M_a = \mathbb{I} \text{ due to } \sum_a p(a) = 1.$$

The evolution of a quantum system A is then

described by a linear map (called quantum channel):

$$E(\rho) = \sum_a p(a) \rho_a = \sum_a p(a) \frac{M_a \rho M_a^\dagger}{p(a)} =$$

$$\Rightarrow E(\rho) = \sum_a M_a \rho M_a^\dagger, \text{ where } \sum_a M_a^\dagger M_a = \mathbb{I}.$$

- Linearity requirement follows from preserving convexity of density operators

$$\begin{aligned} \rho' &= \sum_i p_i \rho'_i = \sum_i p_i \mathcal{E}(\rho_i) \\ &= \mathcal{E}(\rho) = \mathcal{E}\left(\sum_i p_i \rho_i\right) \rightarrow \mathcal{E} \text{ must be a linear map} \end{aligned}$$

- The measurement operators M_a are also called **Kraus operators**. There are $\leq d^2$ Kraus operators, where $d = \dim(A)$.

- Since $\sum_a M_a^\dagger M_a = I$, the map is **trace preserving**

$$\begin{aligned} \text{Tr}[\mathcal{E}(\rho)] &= \text{Tr}\left[\sum_a M_a \rho M_a^\dagger\right] = \\ &= \sum_a \text{Tr}\left[M_a^\dagger M_a \rho\right] = \text{Tr} \rho = 1. \quad \square \end{aligned}$$

\uparrow
 $\sum_a M_a^\dagger M_a = I$

• The map $E(\rho)$ is completely - positive.

(i) A positive map is defined via $E(\rho) \geq 0$ if $\rho \geq 0$.

Proof that : Given arbitrary $|\psi\rangle$, it holds that $\langle \psi | \rho | \psi \rangle \geq 0$.
 E is positive

$$\text{Thus, } \langle \psi | E(\rho) | \psi \rangle = \sum_a \langle \psi | M_a \rho M_a^\dagger | \psi \rangle =$$

$$= \sum_{\mathcal{R}} \sum_a p_{\mathcal{R}} \langle \psi | M_a | \mathcal{R} \rangle \langle \mathcal{R} | M_a^\dagger | \psi \rangle =$$

$$\rho = \sum_{\mathcal{R}} p_{\mathcal{R}} |\mathcal{R}\rangle \langle \mathcal{R}| \quad (\text{spectral decomposition})$$

$$\Rightarrow \langle \psi | E(\rho) | \psi \rangle = \sum_{\mathcal{R}} \sum_a p_{\mathcal{R}} |\langle \psi | M_a | \mathcal{R} \rangle|^2 \geq 0$$

↑ sum of non-negative numbers.

(ii) Completely-positive is a stronger condition than positive.

It requires that the extension of the map

$$E \otimes I : A \otimes E \longmapsto A' \otimes E$$

is positive for any reference (or environment) system E (of arbitrary dimension).

Proof that $E(\rho)$ is completely-positive:

Since M_a are Kraus operators of the positive map

$E : A \rightarrow A'$, we can easily construct Kraus

operators $\{M_a \otimes I_E\}$ for the extended map

$$(E \otimes I_E)(\rho) = \sum_a (M_a \otimes I_E) \rho (M_a^\dagger \otimes I_E),$$

which also fulfill $\sum_a (M_a^\dagger \otimes I_E) (M_a \otimes I_E) = I_A \otimes I_E = I$.

The map $E(\rho) = \sum_a M_a \rho M_a^\dagger$ is therefore completely positive. \square

A quantum channel

$$\mathcal{E}(\rho) = \sum_a M_a \rho M_a^\dagger$$

$$\text{with } \sum_a M_a^\dagger M_a = I$$

This is called the operator-sum representation or Kraus representation of a quantum channel.

The fact that every quantum channel can be expressed in this form is the Choi-Kraus theorem (W.4.4.1).

is therefore a completely-positive trace-preserving linear map, also called CPTP map.

Note that not all positive linear maps are completely positive. One important counter example is the transpose map

$$T : |i\rangle\langle j| \mapsto |j\rangle\langle i|,$$

where $\{|i\rangle\}$ denotes an orthonormal basis (i.e. the computational basis).

$$\text{Thus, } T : \rho \mapsto \rho^T \text{ (or } \rho_{ij} \xrightarrow{T} \rho_{ji} \text{)}$$

" ρ_{ij}^* "

T is positive because

$$\langle \psi | \rho^T | \psi \rangle = \sum_{i,j} \psi_i^* (\rho^T)_{ji} \psi_j =$$

$$= \sum_{i,j} \psi_j^* S_{ij} \psi_i = \sum_{i,j} \psi_i S_{ij} \psi_j^* =$$

$$= \langle \psi^* | S | \psi^* \rangle \text{ for any } |\psi\rangle.$$

If $S \geq 0$ therefore $S^T \geq 0$ as well.

Example for a single qubit:

$$S = \begin{pmatrix} a & b \\ b^* & d \end{pmatrix} \xrightarrow{T} S^T = \begin{pmatrix} a & b^* \\ b & d \end{pmatrix}$$

Eigenvalues of S and S^T are the same.

But, extending T is not necessarily a positive map:

Example of two qubits:

$$T \otimes I : S_{i_1, j_1, i_2, j_2} \mapsto S_{j_1, i_1, i_2, j_2}$$

Consider the maximally entangled state

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}} [|00\rangle + |11\rangle]$$

$$\Rightarrow \mathcal{S} = |\Phi^+\rangle\langle\Phi^+| = \frac{1}{2} \left[|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11| \right]$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \begin{matrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{matrix}$$

Now,

$$\mathcal{S} \xrightarrow{T \otimes I} \frac{1}{2} \left[|00\rangle\langle 00| + |10\rangle\langle 01| + |01\rangle\langle 10| + |11\rangle\langle 11| \right] =$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The eigenvalues of this operator are

$$\lambda_1 = \lambda_2 = \lambda_3 = \frac{1}{2} \text{ and } \lambda_4 = -\frac{1}{2}.$$

This operator is therefore not positive and the transpose map T is thus not completely positive (T is only positive).

Summary, interpretation & freedom of operator-sum representation:

Quantum channel = CPTP map has operator-sum representation

$$\mathcal{E}(\rho) = \sum_{a=1}^{a_{\max} \leq d^2} M_a \rho M_a^\dagger, \quad \sum_a M_a^\dagger M_a = I$$

It arises from unitary U acting on $A \otimes E$ as

$$U: \rho \otimes |0\rangle_E \langle 0|_E \mapsto \sum_a M_a \rho M_a^\dagger \otimes |a\rangle_E \langle a|_E,$$

followed by partial trace on E .

Running this argument backwards, we see that every quantum channel can be realized in this way.

Given $\mathcal{E}(\rho) = \sum_a M_a \rho M_a^\dagger$ with Kraus operators $\{M_a\}$,

we may introduce reference system E with $\dim(E) = a_{\max} = \# \text{Kraus operators}$. A unitary U can be constructed

from the isometry U defined as (Stinespring dilation)

$$U_{AE}: |\psi\rangle_A |0\rangle_E \mapsto \sum_a (M_a |\psi\rangle_A) |a\rangle_E, \quad \sum_a M_a^\dagger M_a = I$$

from which E can be obtained by partial trace on E :

The Kraus operators can thus be written as

$$\langle a | U_{AE} | 0 \rangle_E = M_a .$$

Kraus operator acting on A

Freedom in operator-sum representation:

The operator-sum representation of a given E is

not unique, as we can perform Tr_E in any basis of E .

When expressed in rotated basis

$$|a\rangle = \sum_{\mu} |\mu\rangle V_{\mu a} \quad \text{with unitary } V_{\mu a},$$

the joint state on $A \otimes E$ reads

$$\begin{aligned} \sum_a M_a |\psi\rangle \otimes |a\rangle_E &= \sum_{a, \mu} M_a V_{\mu a} |\psi\rangle |\mu\rangle_E \\ &= \sum_{\mu} N_{\mu} |\psi\rangle |\mu\rangle_E \end{aligned}$$

again if $a_{\max} \neq \mu_{\max}$ the identity $V_{\mu a}$ can be extended to a unitary by appending zeros to the smaller of the two sets of basis states.

with other (equivalent) set of Kraus operators $N_{\mu} = \sum_a V_{\mu a} M_a$.

Any two operator-sums of the same channel \mathcal{E} are related to each other in this way.