Introduction

We saw in the last two lectures how hard it is to distinguish quantum states, but with enough copies we can fully characterise them using state tomography. But once we’ve reconstructed the state that a source produces, how can we measure the similarity between it and another state? For this, we need to consider distance measures, and just like tomography there are two types: Static and Dynamic. Static measures quantify how close two quantum states are and dynamic measures quantify how well information has been preserved during a dynamical process.

1 Static distance measures

1.1 Hamming distance (classical)

The Hamming distance is the number of places at which two bit strings aren’t equal. For example, for the pair

\[ x = 1 1 0 0 \]
\[ y = 0 1 0 1 \]

we have the Hamming distance \( H(x, y) = 2 \). However, in classical information theory we usually deal with a source of information where there’s a probability distribution over some source alphabet. For this case there are more sophisticated distance measures, some of which are introduced next.

1.2 Trace distance (classical)

The trace distance allows us to compare two probability distributions \( \{p_i\} \) and \( \{q_i\} \) over the same index set. It’s defined as

\[ D(p_i, q_i) \equiv \frac{1}{2} \sum_i |p_i - q_i|. \]

Note, there’s no ‘trace’ here, but we call it trace distance in anticipation of the quantum version. In order to justify the use of the word ‘distance’, a distance measure must satisfy the properties of a metric:

1. It must be symmetric \( D(x, y) = D(y, x) \)
2. It must satisfy the triangle inequality \( D(x, z) \leq D(x, y) + D(y, z) \)
3. \( D(x, x) = 0 \)
4. \[ D(x, y) = 0 \rightarrow x = y \]

- Property (1) says that the distance from \( x \) to \( y \) is the same as \( y \) to \( x \). Pretty obvious!
- Property (2) says that the distance from \( x \) to \( z \) (via) \( y \) is at least as great as from \( x \) to \( z \) directly.
- Properties (3) and (4) are trivial!

Here’s an example: In Euclidean two-space, \( \mathbb{R}^2 \), the distance between points/vectors \( p = (x_1, y_1) \) and \( q = (x_2, y_2) \) is \( d(p, q) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} \). This is the shortest distance between two vectors/points. One can see from the figure below that \( d \) satisfies properties (1) and (2) via Pythagoras

\[
\frac{d(x, z)}{d(x, y)} \leq \frac{d(x, y)}{d(y, z)}
\]

which gives
\[
d(x, z) = \sqrt{(d(x, y))^2 + (d(y, z))^2} \leq d(x, y) + d(y, z)
\]

as well as properties (3) and (4) quite easily. One can show using similar techniques that the trace distance is a metric on probability distributions. We’ll see this in a moment for the quantum version, which includes the classical version in the correct limit.

1.3 Fidelity (classical)

Another measure of similarity between two probability distributions is the fidelity

\[
F(p_i, q_i) \equiv \left[ \sum_i \sqrt{p_i q_i} \right]^2
\]

Note that some authors (like Nielsen and Chuang!) use the non-squared version of the fidelity. The difference is just convention. However, most researchers use the squared version I’ve given here. So in any calculations (problem sheets etc.) please use the definitions of quantities given in these notes.

The fidelity can be thought of as the inner product squared between vectors \( p \) and \( q \), whose end points lie on the surface of a unit sphere

\[
p = (\sqrt{p_1}, \sqrt{p_2}, \sqrt{p_3}) \quad q = (\sqrt{q_1}, \sqrt{q_2}, \sqrt{q_3})
\]

where \( p \cdot q = \sum_i \sqrt{p_i q_i} \) and \( \sum_i (\sqrt{p_i})^2 = \sum_i (\sqrt{q_i})^2 = 1 \), c.f. \( r^2 = x^2 + y^2 + z^2 = 1 \).
For \( n \)-dimensional vectors we have the Euclidean vector space \( \mathbb{R}^n \) and the endpoints lie on the unit sphere \( S^{n-1} \) as shown below.

Here, \( \cos \sigma = \frac{p \cdot q}{||p|| \cdot ||q||} \), where \( ||p|| = \sqrt{p \cdot p} \) is the norm or magnitude of the vector. This leads to \( F(p_i, q_i) = \cos^2 \sigma \). Note, the fidelity is not a metric as, for instance, \( F(p_i, p_i) = \sum_i p_i^2 = 1 \), so property (3) isn’t satisfied. But later you’ll see that we can make it into one.

1.4 Trace distance (quantum)

The trace distance between quantum states \( \rho \) and \( \sigma \) is given by

\[
D(\rho, \sigma) = \frac{1}{2} \mathrm{Tr}|\rho - \sigma|,
\]

where \( |A| = \sqrt{A^\dagger A} \) is the positive square root of \( A^\dagger A \). To see the correspondence with the classical version consider that \( \rho \) and \( \sigma \) commute, in which case they’re diagonal in the same basis, \( \rho = \sum_i r_i |i\rangle \langle i| \) and \( \sigma = \sum_i s_i |i\rangle \langle i| \). Then we have that

\[
D(\rho, \sigma) = \frac{1}{2} \mathrm{Tr} \left| \sum_i (r_i - s_i) |i\rangle \langle i| \right| = \frac{1}{2} \mathrm{Tr} \left( \sum_i |r_i - s_i\rangle \langle i| \right) = \frac{1}{2} \sum_i |r_i - s_i|
\]

(7)

Here’s an example

\[
\rho = \frac{2}{3} |0\rangle \langle 0| + \frac{1}{3} |1\rangle \langle 1|, \quad \sigma = \frac{3}{4} |0\rangle \langle 0| + \frac{1}{4} |1\rangle \langle 1|
\]

(9)

leads to

\[
D(\rho, \sigma) = \frac{1}{2} \left( \frac{2}{3} - \frac{3}{4} \right) + \frac{1}{3} - \frac{1}{4} = \frac{1}{2} \left( \frac{1}{12} + \frac{1}{12} \right) = \frac{1}{12}.
\]

(10)

So they’re quite close to each other.

Geometric view (for qubits)

Let \( \rho = \frac{1 + r \sigma}{2} \) and \( \sigma = \frac{1 + s \sigma}{2} \). This gives

\[
D(\rho, \sigma) = \frac{1}{2} \mathrm{Tr}|\rho - \sigma| = \frac{1}{4} \mathrm{Tr}|(r - s) \cdot \sigma|.
\]

(11)
The matrix \(|(r - s) \cdot \sigma|\) has eigenvalues \(\pm |r - s|\) so that

\[
D(\rho, \sigma) = \frac{|r - s|}{2},
\]

(12)

Note that the distance between points in Euclidean space, \(\mathbb{R}^n\), is \(d(r, s) = \sqrt{\sum_{i=1}^{n} |r_i - s_i|^2} = |r - s|\). Thus the trace distance for qubits is half the ordinary Euclidean distance in \(\mathbb{R}^3\) between the vectors describing the states in the Bloch sphere.

So at least for qubits the quantum version of the trace distance is a metric (as it has a one-to-one correspondence with the Euclidean distance) on the space of density operators. How about in general?

- \(D(\rho, \sigma) = 0\) iff \(\rho = \sigma\). Therefore properties (3) and (4) are satisfied.
- \(D(\rho, \sigma) = D(\sigma, \rho)\). Therefore property (1) is satisfied.
- \(D(\rho, \tau) \leq D(\rho, \sigma) + D(\sigma, \tau)\). Therefore property (3) is satisfied.

The last inequality (the triangle inequality) is rather tricky to derive. But it’s informative to go through the steps as the techniques introduced are useful for dealing with calculating the trace distance between arbitrary density matrices (not diagonal in same basis) as we’ll see in an example in the next section. To show the triangle inequality we can use the formula

\[
D(\rho, \sigma) = \max_P \text{Tr}(P(\rho - \sigma)),
\]

(13)

where the maximisation is over all projectors \(P\). To prove the above we can use the relation \(\rho - \sigma = Q - S\), where \(Q\) and \(S\) are positive operators with orthogonal support

\[
\rho - \sigma = UDU^\dagger = U(D^+ + D^-)U^\dagger = UD^+U^\dagger - U\tilde{D}^+U^\dagger = Q - S,
\]

(14)

where \(Q = UD^+U^\dagger\), \(S = U\tilde{D}^+U^\dagger\), \(D^+ (D^-)\) contains all positive (negative) elements of \(D\), and \(\tilde{D}^+ = -D^-\). This means that

\[
|r - s| = Q + S \rightarrow D(\rho, \sigma) = \frac{1}{2} \text{Tr}(Q) + \frac{1}{2} \text{Tr}(S).
\]

(15)

We then have from the property of density matrices \(\text{Tr}(\rho - \sigma) = \text{Tr}(Q - S) = 0\), as \(\text{Tr}(\rho) = \text{Tr}(\sigma) = 1\), which means that \(\text{Tr}(Q) = \text{Tr}(S)\), which then means that

\[
D(\rho, \sigma) = \text{Tr}(Q).
\]

(16)

Before we go any further, I’d just like to mention that Eq. (16) is a very useful formula for calculating the trace distance for two density matrices that aren’t diagonal in the same basis. Ok, so let \(P\) project onto the support of \(Q\), which means that \(\text{Tr}(P(\rho - \sigma)) = \text{Tr}(P(Q - S)) = \text{Tr}(Q) = D(\rho, \sigma)\). Therefore \(D(\rho, \sigma) = \text{Tr}(P(\rho - \sigma))\). Now in general \(P\) can be any projector (not just projecting onto the support of \(Q\)), so we have

\[
\text{Tr}(P(\rho - \sigma)) = \text{Tr}(P(Q - S)) \leq \text{Tr}(PQ) \leq \text{Tr}(Q) = D(\rho, \sigma).
\]

(17)

So there exists a projector \(P\) such that

\[
D(\rho, \tau) = \text{Tr}(P(\rho - \tau)) = \text{Tr}(P(\rho - \sigma) + \text{Tr}(P(\sigma - \tau)) \leq D(\rho, \sigma) + D(\sigma, \tau).
\]

(18)
Thus the trace distance is a metric on the space of density operators. Also, we have that

\[ D(U\rho U^\dagger, U\sigma U^\dagger) = D(\rho, \sigma) \]
\[ D(\mathcal{E}(\rho), \mathcal{E}(\sigma)) \leq D(\rho, \sigma), \tag{19} \]

and many more nice symmetries.

### 1.4.1 Example of trace distance

Let’s take the experiment with photons from the last lecture showing the elements of the reconstructed density matrix for the ideal target state

\[ |\phi_e\rangle = \frac{1}{2} (|0000\rangle + |0011\rangle + |1100\rangle - |1111\rangle)_{1234} \tag{20} \]

Figure 1: Left hand side is the real part and right hand side is the imaginary part. Here the computational basis is represented by the polarization of the photons, \( \{|0\rangle, |1\rangle\} := \{|H\rangle, |V\rangle\} \)

The ideal density matrix looks like this

Figure 2: Ideal density matrix.
and the experimental density matrix looks like this

Figure 3: Part of experimental density matrix (too big to show here!).

The diagonal matrix $D$ looks like this

Figure 4: Diagonal matrix $D$.

and the matrices $U$, $S$ and $Q$ look like

Figure 5: First matrix is $U$, the second is $S$ and the third is $Q$
These are calculated in the program Mathematica, but for qubits you can do them by hand easily. From
the above matrices we have \[ D = \frac{1}{2} \text{Tr} |\rho - \sigma| = \frac{1}{2} \text{Tr}(Q + S) = \frac{1}{2} \text{Tr}(Q) + \frac{1}{2} \text{Tr}(S) = \text{Tr}(Q) = 0.422. \]

### 1.5 Fidelity (quantum)

The fidelity of state \( \rho \) and \( \sigma \) is defined as

\[
F(\rho, \sigma) = \left[ \text{Tr}\left(\sqrt{\rho^{1/2} \sigma \rho^{1/2}}\right) \right]^2,
\]

where \( \rho = \rho^{1/2} \rho^{1/2} = (U \sqrt{D} U^\dagger)(U \sqrt{D} U^\dagger) = U DU^\dagger \), which leads to \( \rho^{1/2} = (U \sqrt{D} U^\dagger) \). Again, when \( \rho \) and \( \sigma \) commute they’re diagonal in the same basis \( \rho = \sum_i |r_i\rangle \langle i| \) and \( \sigma = \sum_i |s_i\rangle \langle i| \), and we have

\[
F(\rho, \sigma) = \left[ \text{Tr}\left(\sqrt{\sum_i r_i s_i |i\rangle \langle i|}\right) \right]^2
= \left[ \text{Tr}\left(\sum_i \sqrt{r_i s_i} |i\rangle\langle i|\right) \right]^2
= \left[ \sum_i \sqrt{r_i s_i} \right]^2
= F(r_i, s_i).
\]  

In the case of a pure state \( |\psi\rangle \) and an arbitrary state \( \sigma \) we have

\[
F(|\psi\rangle, \sigma) = \left[ \text{Tr}\left(|\psi\rangle \langle \sigma| |\psi\rangle \langle \psi|\right) \right]^2
= \left[ \text{Tr}\left(\langle \psi| \sigma |\psi\rangle \right) \right]^2
= \left[ \text{Tr}\left(\langle \psi| \sigma |\psi\rangle \right) \right]^2
= \langle \psi| \sigma |\psi\rangle \equiv \text{Tr}(\sigma |\psi\rangle \langle \psi|)
\]

and for a pure state \( \sigma = |\phi\rangle \langle \phi| \) we have \( F(|\psi\rangle, |\phi\rangle) = |\langle \psi| \phi\rangle|^2 \). Note that again I’m using the squared definition of the fidelity which is the more widely used version (not the same as Nielsen and Chuang!). We also have that

\[
F(U \rho U^\dagger, U \sigma U^\dagger) = F(\rho, \sigma) \quad (23)
F(\mathcal{E}(\rho), \mathcal{E}(\sigma)) \geq F(\rho, \sigma). \quad (24)
\]

While the fidelity is more widely used than the trace distance in the literature for comparing two states, it’s not actually a metric on the space of density operators! However, we can construct a metric from it. To do this we use ‘Uhlmann’s theorem’:

“If \( \rho \) and \( \sigma \) are states of a quantum system \( Q \). Introduce a second quantum system \( R \) which is a copy of \( Q \). Then

\[
F(\rho, \sigma) = \max_{|\phi\rangle, |\psi\rangle} |\langle \psi| \phi\rangle|^2,
\]

\[ 7 \]
where maximisation is over all purifications $|\psi\rangle$ of $\rho$ and $|\varphi\rangle$ of $\sigma$ into $RQ$.

I’m hoping you’ve done purifications! Purification basically means that given a mixed state $\rho_A$ we can always make a pure state by introducing a reference system $R$ (fictitious) of same dimension as $A$ to make $|\psi\rangle_{AR}$, where $\rho_A = \text{Tr}_R(|\psi\rangle_{AR}\langle\psi|)$. One can then show $F(\rho, \sigma) = \max_{|\varphi\rangle} |\langle\psi|\varphi\rangle|^2$, where $|\psi\rangle$ is any fixed purification of $\rho$ and maximisation is over all purifications $|\varphi\rangle$ of $\sigma$. From this it’s perhaps more evident now that $0 \leq F(\rho, \sigma) \leq 1$. To make a metric from the fidelity we define an ‘angle’ between states $\rho$ and $\sigma$ by

$$A(\rho, \sigma) \equiv \cos^{-1}\sqrt{F(\rho, \sigma)}.$$ (26)

We then check the properties of $A$ as a metric:

- $A$ is symmetric in its inputs as the fidelity is (via Uhlmann). Thus, property (1) is satisfied.
- If $\rho = \sigma$, then $F(\rho, \sigma) = 1$ (via Uhlmann), so $A$ is zero. Thus, property (3) is satisfied.
- If $\rho \neq \sigma$, then $|\psi\rangle \neq |\varphi\rangle$ for any purifications of $\rho$ and $\sigma$, so $F(\rho, \sigma) < 1$. Thus, property (4) is satisfied.
- Now we need to prove the triangle inequality...

Let $|\varphi\rangle$ be a purification of $\sigma$ and choose purifications $|\psi\rangle$ of $\rho$ and $|\gamma\rangle$ of $\tau$ such that $F(\rho, \sigma) = |\langle\psi|\varphi\rangle|^2$ and $F(\sigma, \tau) = |\langle\varphi|\gamma\rangle|^2$ and $\langle\psi|\gamma\rangle$ is real and positive (by choosing global phase factors $e^{i\theta}$ for $|\psi\rangle$ and $|\gamma\rangle$). These purifications lie on the surface of the unit sphere $S^{n-1}$, where $n$ is the dimension of $RQ$, as shown in the figure below.

where for $n$-dimensional vectors in $\mathbb{C}^n$ we have $\cos \theta = \frac{|\langle \chi | \zeta \rangle|}{||\chi|| ||\zeta||}$, with $||\chi|| = \sqrt{\langle \chi | \chi \rangle}$ is the norm and $||\chi|| = 1$ for normalised states. The angle between points on the surface of the unit sphere is a metric, therefore

$$\theta_1 \leq \theta_2 + \theta_3$$

$$\cos^{-1}(|\langle \psi | \gamma \rangle|) \leq \cos^{-1}(|\langle \psi | \varphi \rangle|) + \cos^{-1}(|\langle \varphi | \gamma \rangle|)$$

$$\cos^{-1}(|\langle \psi | \gamma \rangle|) \leq A(\rho, \sigma) + A(\sigma, \tau)$$

and by Uhlmann $F(\rho, \tau) \geq |\langle \psi | \gamma \rangle|^2$. Here $|\psi\rangle$ and $|\gamma\rangle$ have been chosen to give the fidelity with respect to $\sigma$ only and therefore we need to maximise to get equality with $F(\rho, \tau)$, thus we have $a \geq$. This means that
Thus, the fidelity can be turned into a metric.

Using the experimental photonic cluster state from the previous section (Section 1.4.1), one finds the fidelity $F = \langle \phi_c \mid \rho_{\exp} \mid \phi_c \rangle = 0.61$ and the fidelity angle $A = \cos^{-1} \sqrt{F} = 38$ degrees.

### 1.6 Trace distance linked to Fidelity

One can show that

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

and for pure states $\rho = \langle \psi \mid \psi \rangle$ with mixed states $\sigma$ we have

$$1 - F(\langle \psi \mid, \sigma) \leq D(\langle \psi \mid, \sigma).$$

Thus the trace distance and the fidelity are quantitatively equivalent measures of closeness for quantum states. We can use either, with the results from one allowing us to deduce equivalent results for the other.

### 2 Dynamic distance measures

What if we’d like to compare how well a channel $\mathcal{E}$ preserves the state $\rho$? It turns out we can use static measures of distances to develop dynamic ones.

#### 2.1 Gate fidelity

Suppose that we try to implement the quantum gate described by the unitary operation $U$ in a quantum computation, but instead implement $\mathcal{E}$, which we hope is a close approximation to $U$. A natural measure of the gate’s success is the gate fidelity

$$F_g(U, \mathcal{E}) \equiv \min_{\mid \psi \rangle} F(U \mid \psi \rangle, \mathcal{E}(\mid \psi \rangle \langle \psi \rangle),$$

where the minimisation is over all possible inputs $\mid \psi \rangle$. For example, if we try to implement the NOT gate, $i.e.$ $X$, but instead do $\mathcal{E}(\rho) = (1 - p)X \rho X + pZ \rho Z$, then we have

$$F_g(X, \mathcal{E}) = \min_{\mid \psi \rangle} \langle \psi \mid X [(1 - p)X \mid \psi \rangle \langle \psi \mid X + pZ \mid \psi \rangle \langle \psi \mid Z \rangle X \mid \psi \rangle$$

$$= \min_{\mid \psi \rangle} [(1 - p) + p \langle \psi \mid Y \mid \psi \rangle^2]$$

$$= 1 - p,$$

where we have used $\langle \psi \mid Y \mid \psi \rangle = 0$ for $\mid \psi \rangle = \mid 0 \rangle$. 


2.2 Entanglement fidelity

Consider the maximally entangled state $|\psi\rangle = \frac{1}{\sqrt{d}} \sum_i |i\rangle |i\rangle$. The entanglement fidelity is defined as

$$F_e(\mathcal{E}) = \langle \psi | (1 \otimes \mathcal{E}) |\psi\rangle |\psi\rangle |\psi\rangle$$

and quantifies the resilience of a maximally entangled state to a unilateral (one-sided) action of the channel $\mathcal{E}$. $F_e(\mathcal{E})$ can be useful in calculating other types of fidelity. For instance

$$\bar{F} = \frac{1}{3} (2F_e(\mathcal{E}) + 1)$$

is the average fidelity resulting from the action of the channel $\mathcal{E}$ on arbitrary input states. Once the set $\{E_i\}$ are known for $\mathcal{E}$, it is easier to calculate $F_e(\mathcal{E})$ rather than $\bar{F}$ directly.

References