Density Matrices

The Schmidt decomposition can also be viewed as a singular value decomposition. Starting from

$$|\Psi_{AB}\rangle = \sum_{i,j} \alpha_{ij} |\psi_i^A\rangle \otimes |\psi_j^B\rangle$$

We view α_{ij} as an $N \times M$ matrix, where $N = \dim(\mathcal{H}_A), M = \dim(\mathcal{H}_B)$.

Since α is not square, it does not in general have an eigendecomposition. But it does have a singular value decomposition, so there exists an $N \times N$ unitary U, an $M \times M$ unitary V, and an $N \times M$ diagonal matrix $\Sigma = \operatorname{diag}(\lambda_1, ..., \lambda_R)$ with nonnegative entries, such that

$$\boldsymbol{\alpha} = U\Sigma V^{\dagger}$$
, $R = \min(N, M)$

These unitaries U,V make the decomposition of $|\Psi_{AB}
angle$ "diagonal",

$$|\Psi_{AB}\rangle = \sum_{i} \lambda_{i} |\phi_{i}^{A}\rangle \otimes |\phi_{i}^{B}\rangle$$

And so the singular values $\{\lambda_i\}$ are the Schmidt coefficients in the Schmidt decomposition, and the SVD provides an alternative to the partial trace for practical computation of the RDM.

Density Matrices

The Schmidt decomposition provides us with out first quantitative definition of entanglement. The number of nonzero Schmidt values is called the **Schmidt rank** χ , and it quantifies entanglement.

$$|\Psi_{AB}\rangle = \sum_{i=1}^{\chi} \sqrt{p_i} |\phi_i^A\rangle \otimes |\phi_i^B\rangle$$

According to our definitions, $|\Psi_{AB}\rangle$ is unentangled if and only if $\chi = 1$. Larger values for χ correspond to states with "more entanglement."

What is the Schmidt rank of the Bell state $|\Phi^+
angle=rac{1}{\sqrt{2}}\left(|00
angle+|11
angle
ight)$? In general when the Schmidt

rank across a cut is equal to the dimension of one of the subsystems, the state is maximally entangled.

Now we can see that $|\Psi_{AB}\rangle$ is entangled if and only if the RDMs ρ_A, ρ_B are impure.

For an quantum subsystem (or equivalently an open quantum system), states are not rays in Hilbert space, but instead are described density matrices.

It will turn out that the evolution of density matrices need not be unitary, but instead belongs to a more general class of physical evolutions called **Quantum Channels**.



In a sense we already understand quantum channels: they all arise by following the evolution of a subsystem when a joint unitary is applied to a joint system.

More formally, a quantum channel maps every valid density matrix to a valid density matrix. So quantum channels should map PSD operators with trace 1 to PSD operators with trace 1.

Density matrices are not only positive operators, they are completely positive, meaning the reduced state of every subsystem is a positive operator.

Mathematically, a **quantum channel** is defined as a *completely positive trace-preserving* linear map. This is the most general kind of evolution that takes all valid density matrices to valid density matrices.

In general, the input and output of a quantum channel need not have the same dimension. If I send you 10 qubits and you receive 3 of them, we are communicating through a quantum channel.

In a sense we already understand quantum channels: they all arise by following the evolution of a subsystem when a joint unitary is applied to a joint system.

What quantum channel arises on subsystem A in the joint evolution: $\Lambda(X) (H \otimes I) |00\rangle = |\Phi^+\rangle$?



We have $\rho_A(0) = |0\rangle\langle 0|$, $\rho_A(t) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$. The channel took us from 0 to an equal mixture of 0 and 1.

Suppose we act with the same unitary on a different initial state: $\Lambda(X) (H \otimes I) |11\rangle = |\Psi^-\rangle$?



Now we have $\rho_A(0) = |1\rangle\langle 1|$, $\rho_A(t) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$. The channel took us from 1 to an equal mixture of 0 and 1.

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Compare it to the stochastic matrix that scrambles deterministic bits into fair coins!

$$\begin{bmatrix} 1\\0 \end{bmatrix} \text{ or } \begin{bmatrix} 0\\1 \end{bmatrix} - \begin{bmatrix} 1/2 & 1/2\\1/2 & 1/2 \end{bmatrix} - \begin{bmatrix} 1/2\\1/2 \end{bmatrix}$$

Quantum channels describe the evolution of probability distributions of quantum states, so it is no surprise that they include stochastic maps as a subset.

The classical probability distributions we discussed before, for example defined on the space of n bit strings, can be represented as density matrices:

$$\rho = \sum_{x \in \{0,1\}^n} \pi_x |x\rangle \langle x|$$

Density matrices like this which can be written as a probability distributions of unentangled states are called **separable states**. They have the general form:

$$\rho = \sum_{k} \pi_{k} |a_{k}\rangle \langle a_{k}| \otimes |b_{k}\rangle \langle b_{k}|$$

Note that these states do not always have the form $\rho_A \otimes \rho_B$. The reason is that $\rho_A \otimes \rho_B$ does not allow for any correlations at all – not even classical correlations.

To derive the general form of a quantum channel, suppose we start with a state in a Hilbert space $\mathcal{H}_{sys} \otimes \mathcal{H}_{env}$ that is initially uncorrelated between the system and the environment:

 $\rho_{SE}(0) = \rho_{\rm sys}(0) \otimes \rho_{\rm env}(0)$

Suppose further that environment is large and isolated, so it is initially in a pure state:

 $\rho_{SE}(0) = \rho_{\rm sys}(0) \otimes |0_E\rangle \langle 0_E|$

The evolution of the full system + environment proceeds by some joint unitary U

 $\rho_{SE}(t) = U\left(\rho_{\rm sys}(0) \otimes |0_E\rangle \langle 0_E|\right) U^{\dagger}$

Then we trace out the environment to obtain a quantum channel \mathcal{E} acting on the system:

$$\mathcal{E}(\rho_{\rm sys}(0)) = \rho_{\rm sys}(t) = \operatorname{tr}_{\rm env}\rho_{SE}(t) = \operatorname{tr}_{\rm env}\left[U\left(\rho_{\rm sys}(0)\otimes|0_E\rangle\langle 0_E|\right)U^{\dagger}\right]$$

To derive the general form of a quantum channel, suppose we start with a state that is initially uncorrelated between the system and the environment, then act on the system with a joint unitary, then trace out the environment:

 $\mathcal{E}(\rho_{\rm sys}(0)) = \operatorname{tr}_{\rm env} \left[U\left(\rho_{\rm sys}(0) \otimes |0_E\rangle \langle 0_E|\right) U^{\dagger} \right]$ $= \sum_k \langle k_E | U | 0_E \rangle \rho_{\rm sys}(0) \langle 0_E | U^{\dagger} | k_E \rangle$

Where $\{|k_E\rangle\}$ is a basis for the \mathcal{H}_{env} , and $E_k = \langle k_E | U | 0_E \rangle$ is an **operator** that acts on \mathcal{H}_{sys} .

Now defining $\rho = \rho_{sys}(0)$ (since our initial state was arbitrary) we have expressed the channel as:

$$\mathcal{E}(\rho) = \sum_{k} \langle k_E | U | 0_E \rangle \rho \langle 0_E | U^{\dagger} | k_E \rangle = \sum_{k} E_k \rho E_k^{\dagger}$$

This expression is called the **operator-sum representation** of the quantum channel:

$$\mathcal{E}(\rho) = \sum_{k} E_k \rho E_k^{\dagger}$$

And the operators $\{E_k\}$ are called **Krauss operators**. Explicit forms for these operators can be found by modeling the environment, or taking input from experiment (just as in the case of Hamiltonians), or else they arise from some known measurements on the system.

From our previous calculation, note that the Krauss operators satisfy a **completeness relation**:

$$\sum_{k} E_{k}^{\dagger} E_{k} = \langle 0_{E} | U^{\dagger} | k_{E} \rangle \langle k_{E} | U | 0_{E} \rangle = I$$

We have shown that any quantum channel has a Krauss operator-sum representation:



Moreover, it can be shown that any collection of linear operators $\{E_k\}$ satisfying the completeness relation above maps every valid density matrix to a valid density matrix. Hence any \mathcal{E} of the form above will be a valid quantum channel.

Our first example of a quantum channel describes measuring a state $|\psi
angle$.

Recall that given a basis of events $\{|a_k\rangle\}$, a measurement outcome a_k indicates that the state of the system is projected onto the corresponding $|a_k\rangle$

$$\psi\rangle \to \frac{\langle\psi|a_k\rangle}{|\langle\psi|a_k\rangle|}|a_k\rangle$$

Expressed in terms of density matrices $ho = |\psi\rangle\langle\psi|$ and projectors $\Pi_k = |a_k\rangle\langle a_k|$, this becomes

$$\rho \to \frac{\Pi_k \rho \Pi_k}{\operatorname{tr} \left(\Pi_k \rho \right)}$$

Where $tr(\Pi_k \rho)$ is the probability of obtaining outcome k.

If we consider the full basis of events $\{|a_k\rangle\}$, then the set of projectors $\Pi_k = |a_k\rangle\langle a_k|$ form a set of Krauss operators because they satisfy the completeness relation:

$$\sum_{k} \Pi_{k}^{\dagger} \Pi_{k} = \sum_{k} \Pi_{k}^{2} = \sum_{k} \Pi_{k} = I$$

Therefore the measurement itself can be expressed as a quantum channel with $E_k = E_k^{\dagger} = \Pi_k$:

$$\mathcal{E}(\rho) = \sum_{k} \Pi_{k} \rho \Pi_{k}$$

Which is a new density matrix that assigns a probability $\operatorname{tr}(\Pi_k \rho)$ to the state $\frac{\Pi_k \rho \Pi_k}{\operatorname{tr}(\Pi_k \rho)}$.

Next we will describe three ubiquitous single-qubit quantum channels that describe noisy systems.

Unlike the case of single-qubit unitaries, which are just a prelude for multi-qubit unitaries, we can already describe interesting physical scenarios by single-qubit channels that are used repeatedly.

For example, Alice could produce a quantum state of many qubits, and then transmit them to Bob one at a time through a noisy transmission line.

Alternatively, Alice may prepare her state of many qubits and then worry about it slowly being corrupted by the environment. If the environment acts independently on each qubit then we can model this by a product of single-qubit quantum channel.

Our first example of a qubit channel is called the **depolarizing channel**, and it captures the notion of a random Pauli error occurring on our qubit.

With probability 1 – p the state is unchanged, and with probability p we apply one of X, Y, Z at random.

Since each density matrix is mapped to a mixture of 4 possible density matrices, we have

$$\mathcal{E}(\rho) = (1-p)\rho + \frac{p}{3}\left(X\rho X + Y\rho Y + Z\rho Z\right)$$

which is the Krauss operator-sum representation of the depolarizing channel.

To understand the effect of sending a qubit through a **depolarizing channel**, use the Bloch sphere:

$$\rho = \frac{1}{2} \left(I + \vec{\alpha} \cdot \vec{\sigma} \right)$$

Where direct calculation shows

$$\mathcal{E}(\rho) = (1-p)\rho + \frac{p}{3}(X\rho X + Y\rho Y + Z\rho Z) = (1 - \frac{4}{3}p)\rho + \frac{4}{3}pI$$

Which can be interpreted as either keeping ρ , or discarding it and replacing it with the maximally mixed state. This equivalence (random Pauli vs replace with mixed state) can be a little confusing.

From the Bloch sphere point of view, we replace $\vec{\alpha} \to \vec{\alpha} \left(1 - \frac{4}{3}p\right)$, and so the volume of the block

ball is shrinking. Recall that pure states are on the surface of the ball, so the depolarizing channel increases the impurity of the state with each application, until there is nothing left but the identity.

The channel we will consider is the **dephasing channel**, which represents the leakage of information to the environment. The unitary map on the system + environment is

$$|0\rangle_s \mapsto \sqrt{1-p}|0\rangle_s|0\rangle_e + \sqrt{p}|0\rangle_s|1\rangle_e$$

$$|1\rangle_s \mapsto \sqrt{1-p}|1\rangle_s|0\rangle_e + \sqrt{p}|1\rangle_s|2\rangle_e$$

To unpack this, note that there is a preferred basis $\{0,1\}$ which the environment learns about. The environment does not flip the state (the unitary above never sends $|0\rangle_s$ to $|1\rangle_s$).

With probability 1 - p, the environment remains in the $|0\rangle_e$ state. With probability p, the state of the environment changes depending on whether the system is a $|0\rangle_s$ or $|1\rangle_s$.

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The Krauss operators for the **dephasing channel** can therefore be computed:

$$E_0 = \langle 0_E | U | 0_E \rangle = \sqrt{1 - p}I$$
$$E_1 = \langle 1_E | U | 0_E \rangle = \sqrt{p} | 0 \rangle \langle 0 |$$
$$E_2 = \langle 2_E | U | 0_E \rangle = \sqrt{p} | 1 \rangle \langle 1 |$$

This is a good point to mention the fact that the representation of a given channel in terms of Krauss operators is not unique. Actually, we already saw this with the depolarizing channel.

Expressing
$$E_1, E_2$$
 in the equivalent form, $E_1 = \frac{\sqrt{p}}{2} (I+Z)$, $E_2 = \frac{\sqrt{p}}{2} (I-Z)$, we find

$$\mathcal{E}(\rho) = \sum_{k} E_{k} \rho E_{k}^{\dagger} = \left(1 - \frac{p}{2}\right)\rho + \frac{p}{2}Z\rho Z$$

Therefore the **dephasing channel** is equivalent to applying a Pauli Z error with probability p/2.

$$\mathcal{E}(\rho) = \sum_{k} E_k \rho E_k^{\dagger} = \left(1 - \frac{p}{2}\right)\rho + \frac{p}{2}Z\rho Z$$

This has the effect of shrinking the off-diagonal density matrix elements in the 0/1 basis:

$$\mathcal{E}\begin{bmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{bmatrix} = \begin{bmatrix} \rho_{00} & (1-p)\rho_{01} \\ (1-p)\rho_{10} & \rho_{11} \end{bmatrix}$$

Therefore after many applications of the channel, the off-diagonal terms will be gone and we'll have a mixture in the computational basis:

$$\mathcal{E}^{T}(\rho) \approx p_{00}|0\rangle\langle 0| + p_{11}|1\rangle\langle 1|$$

Dephasing (in the computational basis) turns quantum superpositions into mixtures of computational basis states --- which are separable states with no entanglement.

A mixture of computational basis states is simply a classical probability distribution. This transition from quantum information to classical information is called **decoherence**.

The idea that leaking information to the environment can turn a quantum superposition into a classical mixture is the modern explanation for apparently non-unitary measurement effects in QM.

Instead of saying that measurements instantly update a state, we can say that a joint unitary entangles the system with its environment (a measurement apparatus). Failing to track all the degrees of freedom in the environment (perhaps because it is macroscopic) leads to these DoF being traced out, which causes decoherence and "collapses" the quantum superposition.

The last example we will use to gain a feel for quantum channels is the **amplitude-damping channel**. It represents the "relaxation" of a qubit into the state $|0\rangle$.

The "0" and "1" states in a classical transistor correspond to measurably distinct voltages. If "1" is the higher energy state, we might worry about spontaneous relaxations down to the "0" state. This is relevant for qubit implementations including "superconducting transmons" built at IBM, Google, etc.

Since the evolution on the joint system needs to be unitary, the environment must record the decay of $|1\rangle$ to $|0\rangle$ every time it happens. We can think of this as the energy lost to the environment,

$$\begin{split} |0\rangle_s &\mapsto |0\rangle_s |0\rangle_e \\ |1\rangle_s &\mapsto \sqrt{1-p} |1\rangle_s |0\rangle_e + \sqrt{p} |0\rangle_s |1\rangle_e \end{split}$$

Tracing out the environment yields the Krauss representation of the amplitude-damping channel,

$$E_0 = \langle 0_E | U | 0_E \rangle = | 0 \rangle \langle 0 | + \sqrt{1 - p} | 1 \rangle \langle 1 |$$

$$E_1 = \langle 1_E | U | 0_E \rangle = \sqrt{p} | 1 \rangle \langle 1 |$$

Which we can use to compute its action on an arbitrary density matrix:

$$\mathcal{E}\begin{bmatrix}\rho_{00} & \rho_{01}\\\rho_{10} & \rho_{11}\end{bmatrix} = \begin{bmatrix}\rho_{00} + p\rho_{11} & \sqrt{1-p}\rho_{01}\\\sqrt{1-p}\rho_{10} & (1-p)\rho_{11}\end{bmatrix}$$

As expected, after many applications of the amplitude-damping channel we obtain the state $|0\rangle\langle 0|$.

We may also define continuous versions of all these channels by applying them L times with $p = L^{-1}$. In the limit $L \to \infty$ this leads to exponential decays of density matrix elements.