Uhlmann’s Theorem

Formal statement

Let $\rho_{(A)}$ and $\sigma_{(A)}$ be density operators on a finite-dimensional Hilbert space mathcal $H_{(A)}$. Define the root fidelity by

$$F(\rho_A, \sigma_A) = \left\| \sqrt{\rho_A}\sqrt{\sigma_A} \right\|_1 = \operatorname{Tr}\sqrt{\sqrt{\rho_A}\sigma_A\sqrt{\rho_A}}.$$

Here \|X\|$_1$=Tr√(X^† X) is the trace norm. Uhlmann’s theorem says that

$$F(\rho_A, \sigma_A) = \max_{|\psi_\rho\rangle, |\psi_\sigma\rangle} \left| \langle \psi_\rho | \psi_\sigma \rangle \right|,$$

where the maximum is over all purifications $|\psi\rho\rangle_{(AR)}$ of $\rho_{(A)}$ and all purifications $|\psi\sigma\rangle_{(AR)}$ of $\sigma_{(A)}$ on a common reference system R large enough to purify both states. Equivalently, one may fix any purification $|\psi\rho\rangle_{(AR)}$ of $\rho_{(A)}$, and maximize only over purifications $|\psi\sigma\rangle_{(AR)}$ of $\sigma_{(A)}$:

$$F(\rho_A, \sigma_A) = \max_{|\psi_\sigma\rangle:\, \operatorname{Tr}_R |\psi_\sigma\rangle\langle\psi_\sigma| = \sigma_A} \left| \langle \psi_\rho | \psi_\sigma \rangle \right|.$$

Some books use the squared fidelity convention

$$F_{\mathrm{sq}}(\rho_A, \sigma_A) = \left(\operatorname{Tr}\sqrt{\sqrt{\rho_A}\sigma_A\sqrt{\rho_A}} \right)^2.$$

With that convention, Uhlmann’s theorem is written as

$$F_{\mathrm{sq}}(\rho_A, \sigma_A) = \max_{|\psi_\rho\rangle, |\psi_\sigma\rangle} \left| \langle \psi_\rho | \psi_\sigma \rangle \right|^2.$$

Both forms express the same theorem; the only difference is whether fidelity means overlap or squared overlap.

Meaning before the proof

For pure states, the natural measure of similarity is the absolute inner product. If

$$\rho = |\psi\rangle\langle\psi|, \qquad \sigma = |\phi\rangle\langle\phi|,$$

then

$$F(\rho, \sigma) = |\langle\psi|\phi\rangle|.$$

The problem is that mixed states do not have state vectors. A mixed state is a density operator, not a ray in Hilbert space, so it is not obvious what "overlap" should mean.

The purification theorem gives a way out. Every mixed state can be regarded as the shadow of a pure state on a larger system. Uhlmann's theorem says that the correct mixed-state fidelity is exactly the largest possible pure-state overlap between such enlarged descriptions. In other words, two mixed states are close when their purifications can be chosen to be close.

The operational mental image is this: $\rho_{(A)}$ and $\sigma_{(A)}$ are two shadows on system A. A purification is one possible three-dimensional object casting the shadow. Uhlmann's theorem says that the similarity of the shadows is the best possible similarity of the objects, after we are allowed to rotate and relabel the hidden reference system.

Proof

Choose a reference Hilbert space mathcal $H_{(R)}$ with dimension at least dimmathcal $H_{(A)}$. Fix an orthonormal basis \|j⟩$_{(R)}$\ of the reference and an isomorphic basis \|j⟩$_{(A)}$\ of A. Define the unnormalized maximally entangled vector

$$|\Omega\rangle_{AR} = \sum_j |j\rangle_A |j\rangle_R.$$

The canonical purification of $\rho_{(A)}$ is

$$|\psi_\rho\rangle_{AR} = (\sqrt{\rho_A} \otimes I_R)|\Omega\rangle_{AR},$$

and similarly

$$|\psi_\sigma\rangle_{AR} = (\sqrt{\sigma_A} \otimes I_R)|\Omega\rangle_{AR}.$$

These are normalized because $\mathrm{Tr}\rho_A = \mathrm{Tr}\sigma_A = 1$, and tracing out R gives ρ_A and σ_A, respectively.

By the uniqueness of purification, every purification of σ_A on the same sufficiently large reference system can be written as

$$(I_A \otimes U_R)|\psi_\sigma\rangle_{AR}$$

for some unitary U_R, up to irrelevant unused dimensions. Therefore, if we fix $|\psi_\rho\rangle$, the optimization over purifications of σ_A becomes an optimization over reference unitaries:

$$\max_{|\phi_\sigma\rangle} |\langle\psi_\rho|\phi_\sigma\rangle| = \max_U |\langle\psi_\rho|(I_A \otimes U_R)|\psi_\sigma\rangle| \,.$$

Using the standard vectorization identity, this inner product can be written as

$$\langle\psi_\rho|(I_A \otimes U_R)|\psi_\sigma\rangle = \mathrm{Tr}\left(\sqrt{\rho_A}\sqrt{\sigma_A}\,U^T\right),$$

where the transpose depends only on the chosen reference basis. Since U ranges over all unitaries, so does U^T. Hence the optimization is equivalent to

$$\max_U |\mathrm{Tr}\,(\sqrt{\rho_A}\sqrt{\sigma_A}\,U)| \,.$$

Now we use the variational characterization of the trace norm:

$$\|X\|_1 = \max_U |\,\mathrm{Tr}(XU)|,$$

where the maximum is over all unitaries of the appropriate dimension. Applying this to

$$X = \sqrt{\rho_A}\sqrt{\sigma_A},$$

we obtain

$$\max_U |\mathrm{Tr}\,(\sqrt{\rho_A}\sqrt{\sigma_A}\,U)| = \|\sqrt{\rho_A}\sqrt{\sigma_A}\|_1 \,.$$

By definition, the right-hand side is

$$F(\rho_A, \sigma_A).$$

Therefore

$$F(\rho_A, \sigma_A) = \max_{|\psi_\rho\rangle, |\psi_\sigma\rangle} |\langle\psi_\rho|\psi_\sigma\rangle|.$$

This proves Uhlmann's theorem.

Why the proof works

The proof has two moving parts. The first is uniqueness of purification. Once one purification of σ(A) is chosen, every other purification of σ(A) is obtained by changing only the reference system. Thus, the search over purifications becomes a search over reference unitaries.

The second is polar decomposition, hidden inside the trace-norm identity. The operator

$$\sqrt{\rho_A}\sqrt{\sigma_A}$$

is generally not positive and not Hermitian. It has a "magnitude" and a "phase," just as a complex number has modulus and phase. The reference unitary is chosen to cancel the phase and align the purifications as well as possible. After that alignment, the largest overlap is exactly the trace norm.

This is the geometric content of the theorem. Fidelity is the best possible coherent alignment between purifications.

Example 1: pure states

Let

$$\rho = |\psi\rangle\langle\psi|, \qquad \sigma = |\phi\rangle\langle\phi|.$$

Since these states are already pure, no nontrivial reference system is needed. Their purifications can be chosen as

$$|\psi\rangle_A|0\rangle_R, \qquad |\phi\rangle_A|0\rangle_R.$$

Their overlap is

$$\langle\psi|\phi\rangle.$$

So Uhlmann's theorem gives

$$F(\rho,\sigma) = |\langle\psi|\phi\rangle|.$$

This confirms that mixed-state fidelity really extends the familiar pure-state overlap. For pure states, there is no hidden reference system to optimize over.

Example 2: commuting classical states

Suppose

$$\rho = \sum_i p_i|i\rangle\langle i|, \qquad \sigma = \sum_i q_i|i\rangle\langle i|.$$

These two states commute and are diagonal in the same basis. Then

$$\sqrt{\rho}\sqrt{\sigma} = \sum_i \sqrt{p_i q_i}|i\rangle\langle i|,$$

so

$$F(\rho,\sigma) = \sum_i \sqrt{p_i q_i}.$$

This is the classical Bhattacharyya coefficient between probability distributions p\ and q. Thus Uhlmann's theorem contains the classical notion of distributional overlap as a special case.

For example, if

$$p = (0.9, 0.1), \qquad q = (0.5, 0.5),$$

then

$$F(\rho,\sigma) = \sqrt{0.9\cdot 0.5} + \sqrt{0.1\cdot 0.5} \approx 0.8944.$$

With the squared convention, the fidelity would be

$$F_{\mathrm{sq}}(\rho,\sigma) \approx 0.8.$$

The operational image is simple: when two states are diagonal in the same basis, the best purification overlap is obtained by pairing the same classical labels with the same reference labels.

Example 3: a pure state versus a maximally mixed state

Let

$$\rho = |0\rangle\langle 0|, \qquad \sigma = \frac{I}{2}.$$

Using the formula,

$$F(\rho,\sigma) = \sqrt{\langle 0|\sigma|0\rangle} = \frac{1}{\sqrt{2}}.$$

A purification of ρ is

$$|0\rangle_A|0\rangle_R.$$

A purification of σ is the Bell state

$$|\Phi^+\rangle_{AR} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}.$$

Their overlap is

$$\left|\langle 0|_A\langle 0|_R \frac{|00\rangle + |11\rangle}{\sqrt{2}}\right| = \frac{1}{\sqrt{2}}.$$

Thus this Bell purification already achieves the Uhlmann maximum. The interpretation is that the maximally mixed state has only half of its purified amplitude aligned with $|0\rangle$; the other half lies in an orthogonal branch.

Example 4: orthogonal states

Let

$$\rho = |0\rangle\langle 0|, \qquad \sigma = |1\rangle\langle 1|.$$

Then

$$\sqrt{\rho}\sqrt{\sigma} = |0\rangle\langle 0|1\rangle\langle 1| = 0,$$

so

$$F(\rho, \sigma) = 0.$$

No matter how we purify these states, their purifications cannot be made to overlap. The reason is that the reduced states already live on orthogonal supports. The reference system can rotate hidden labels, but it cannot make orthogonal visible states on A become nonorthogonal.

This example is useful because it shows the boundary of reference-system freedom. Uhlmann optimization can align hidden systems, but it cannot change the observable support structure on A.

Example 5: equal states

If

$$\rho = \sigma,$$

then clearly

$$F(\rho, \sigma) = 1.$$

Uhlmann's theorem explains this geometrically. Choose the same purification for both states. Then the overlap is exactly one. Conversely, if the maximum purification overlap is one, then two purifications can be chosen to be the same vector up to a global phase. Tracing out the reference then gives the same reduced state, so $\rho=\sigma$.

Thus fidelity equals one exactly when the states are identical.

How the theorem is used

Uhlmann's theorem is useful because it turns a mixed-state problem into a pure-state geometry problem. If one wants to prove a property of fidelity, one can often purify the states, use ordinary inner-product geometry, and then optimize over the reference system.

It is also the conceptual basis of the Bures angle and Bures distance. The Bures angle is often written as

$$A(\rho,\sigma)=\arccos F(\rho,\sigma),$$

using the root-fidelity convention. Uhlmann's theorem says that this is the smallest possible Hilbert-space angle between purifications of ρ and σ. Thus the geometry of mixed states is inherited from the geometry of pure states, after minimizing over the unobserved reference degrees of freedom.

In quantum information, this viewpoint is used in continuity bounds, quantum error correction, decoupling, cryptographic security, channel-state duality, and one-shot information theory. Whenever a theorem says that a real implementation is close to an ideal state, fidelity is often the quantity that measures this closeness. Uhlmann's theorem then says that closeness of mixed states is equivalent to closeness of suitable purifications.

Common mistakes

The most common mistake is to confuse the two fidelity conventions. With the root convention,

$$F(\rho,\sigma)=\|\sqrt{\rho}\sqrt{\sigma}\|_1$$

and Uhlmann's theorem gives a maximum absolute inner product. With the squared convention,

$$F_{\mathrm{sq}}(\rho, \sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_1^2$$

and Uhlmann's theorem gives a maximum squared inner product. Both are used in the literature, so one must check the convention before comparing formulas.

A second mistake is to think that the theorem says arbitrary purifications have overlap equal to fidelity. That is false. Uhlmann's theorem says the fidelity is the maximum overlap after optimizing over purifications. Badly chosen purifications can have smaller overlap.

A third mistake is to forget that the optimizing freedom lives only on the reference system. We are not allowed to change $\rho_{(A)}$ or $\sigma_{(A)}$. We are only allowed to choose how their purifying systems are represented.

Final mental image

The purification theorem says that every mixed state is the shadow of a pure state on a larger Hilbert space. The uniqueness of purification says that the shadow determines the pure state up to an isometry on the hidden reference. Uhlmann's theorem adds the metric statement: the fidelity between two shadows is the best possible overlap between the pure states that cast them.

In one sentence:

$$\text{mixed-state fidelity} = \text{maximum pure-state overlap after optimally aligning the r}$$

This is why Uhlmann's theorem connects fidelity, geometry, and purification. Fidelity is not merely an algebraic trace formula. It is the visible-system remnant of ordinary Hilbert-space angle after the invisible reference systems have been optimally aligned.

References

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