University of Oslo

FYS3415/FYS4415 — Quantum computing and quantum information

Problem set 9

This problem set will be discussed on **Apr. 15**.

Problem 1: Trace Distance

For two quantum states ρ and σ, the trace distance is defined by

$$D(\rho,\sigma) = \frac{1}{2}\operatorname{Tr}|\rho-\sigma|.$$

a) Warm-up computation.

Consider the two single-qubit states

$$\rho = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}, \qquad \sigma = |+\rangle\langle+| = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}.$$

Calculate the trace distance $D(\rho,\sigma)$.

Solution: The difference matrix is

$$\Delta = \rho - \sigma = \begin{pmatrix} 1/4 & -1/2 \\ -1/2 & -1/4 \end{pmatrix}.$$

Its characteristic equation is $\lambda^2 - \frac{5}{16} = 0$, so the eigenvalues are $\lambda_\pm = \pm\frac{\sqrt{5}}{4}$. Therefore

$$D(\rho,\sigma) = \frac{1}{2}\operatorname{Tr}|\rho-\sigma| = \frac{1}{2}\left(\left|\frac{\sqrt{5}}{4}\right| + \left|-\frac{\sqrt{5}}{4}\right|\right) = \frac{\sqrt{5}}{4}.$$

b) Maximum projector.

In lecture you proved that for any two states ρ,σ,

$$D(\rho,\sigma) = \max_{0\le E\le I} \operatorname{Tr}(E(\rho-\sigma)),$$

where the maximum is over all POVM elements E. Let $|e_+\rangle$ be the eigenvector of $\rho-\sigma$ corresponding to the positive eigenvalue, and let $P_+ = |e_+\rangle\langle e_+|$.

Verify that

$$\operatorname{Tr}(P_+(\rho-\sigma)) = D(\rho,\sigma).$$

Solution: Let $\Delta = \rho - \sigma$. Its spectral decomposition is

$$\Delta = \lambda_+ |e_+\rangle\langle e_+| + \lambda_- |e_-\rangle\langle e_-|, \qquad \lambda_+ = \frac{\sqrt{5}}{4}, \quad \lambda_- = -\frac{\sqrt{5}}{4}.$$

Writing also $P_- = |e_-\rangle\langle e_-|$, we get

$$\operatorname{Tr}(P_+\Delta) = \operatorname{Tr}\big(P_+(\lambda_+P_+ + \lambda_-P_-)\big) = \lambda_+\operatorname{Tr}(P_+) + \lambda_-\operatorname{Tr}(P_+P_-) = \lambda_+ = \frac{\sqrt{5}}{4} = D(\rho,\sigma).$$

Thus P_+ attains the maximum in the formula above.

Problem 2: Fidelity and Uhlmann's theorem

The *fidelity* of density operators ρ and σ is

$$F(\rho,\sigma) \equiv \mathrm{Tr}\sqrt{\sqrt{\rho}\,\sigma\,\sqrt{\rho}}.$$

It is not a metric, but it measures similarity: $F(\rho,\sigma) = 1$ iff $\rho = \sigma$, and $F(\rho,\sigma) = 0$ iff the supports of ρ and σ are orthogonal.

In this problem you prove basic properties of fidelity and derive Uhlmann's theorem.

a) Special cases.

i) Let $\rho_\psi = |\psi\rangle\langle\psi|$ be a pure state. Show that for any density operator ρ,

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

ii) Let

$$\rho = \sum_i r_i\,|i\rangle\langle i|, \qquad \sigma = \sum_i s_i\,|i\rangle\langle i|$$

be commuting density operators. Show that

$$F(\rho,\sigma) = \sum_i \sqrt{r_i s_i}.$$

iii) Compute the fidelity between

$$\rho = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}, \qquad \sigma = \frac{1}{2}I.$$

Solution: i) Since $\rho_\psi^2 = \rho_\psi$, we have

$$\sqrt{\rho_\psi}\,\rho\,\sqrt{\rho_\psi} = \rho_\psi\rho\rho_\psi = \langle\psi|\rho\,|\psi\rangle\,\rho_\psi.$$

Therefore

$$F(\rho_\psi,\rho) = \mathrm{Tr}\sqrt{\langle\psi|\rho\,|\psi\rangle\,\rho_\psi} = \sqrt{\langle\psi|\rho\,|\psi\rangle}.$$

ii) Since ρ and σ are diagonal in the same basis,

$$\sqrt{\rho}\,\sigma\,\sqrt{\rho} = \sum_i r_i s_i\,|i\rangle\langle i|,$$

so

$$F(\rho,\sigma) = \mathrm{Tr}\left(\sum_i \sqrt{r_i s_i}\;|i\rangle\langle i|\right) = \sum_i \sqrt{r_i s_i}.$$

iii) By (ii),

$$F(\rho,\sigma) = \sqrt{\tfrac{3}{4}\cdot\tfrac{1}{2}} + \sqrt{\tfrac{1}{4}\cdot\tfrac{1}{2}} = \sqrt{\tfrac{3}{8}} + \sqrt{\tfrac{1}{8}} = \frac{\sqrt{3}+1}{2\sqrt{2}}.$$

b) Key lemma.

Show that for any operator A,

$$\max_U |\operatorname{Tr}(UA)| = \operatorname{Tr}|A|,$$

where $|A| = \sqrt{A^\dagger A}$ and the maximum is over all unitaries U. Hint[1].

Solution: Write

$$A = V|A|$$

using the polar decomposition, where $|A| = \sqrt{A^\dagger A} \geq 0$, and V is unitary after extending the partial isometry on the support of $|A|$ arbitrarily to its orthogonal complement.

Now diagonalize $|A|$:

$$|A| = \sum_i s_i |i\rangle\langle i|, \qquad s_i \geq 0.$$

Then for any unitary U,

$$\begin{aligned}
|\operatorname{Tr}(UA)| &= |\operatorname{Tr}(UV|A|)| \\
&= \left|\sum_i \langle i|UV|A|\,|i\rangle\right| \\
&= \left|\sum_i s_i \langle i|UV\,|i\rangle\right| \\
&\leq \sum_i s_i\,|\langle i|UV\,|i\rangle| \\
&\leq \sum_i s_i \\
&= \operatorname{Tr}|A|.
\end{aligned}$$

Here we used that UV is unitary, so each diagonal entry satisfies

$$|\langle i|UV\,|i\rangle| \leq 1.$$

To achieve equality, choose

$$U = V^\dagger.$$

Then

$$|\operatorname{Tr}(UA)| = \operatorname{Tr}|A|.$$

Therefore

$$\max_U |\operatorname{Tr}(UA)| = \operatorname{Tr}|A|.$$

c) Uhlmann's theorem.

Let ρ and σ be density operators on a system Q. Uhlmann's theorem states that

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

where the maximum is over all purifications $|\psi\rangle$ of ρ and $|\phi\rangle$ of σ onto $Q \otimes R$, with $R \cong Q$.

[1] Use the polar decomposition $A = V|A|$ for unitary V, and diagonalize $|A|$.

Prove this in the following steps.

i) Fix an orthonormal basis $\{|i\rangle\}$ of Q, use the corresponding basis on R, and define

$$|\Omega\rangle_{QR} = \sum_i |i\rangle_Q |i\rangle_R, \qquad |\psi_0\rangle_{QR} = (\sqrt{\rho} \otimes I_R)|\Omega\rangle, \qquad |\phi_0\rangle_{QR} = (\sqrt{\sigma} \otimes I_R)|\Omega\rangle.$$

Show that $|\psi_0\rangle$ and $|\phi_0\rangle$ are purifications of ρ and σ. Conclude that every purification of ρ onto $Q \otimes R$ has the form $(I_Q \otimes U_R)|\psi_0\rangle$ for some unitary U_R on R, and similarly for σ.

ii) Using

$$\langle\Omega|(A \otimes B)|\Omega\rangle = \mathrm{Tr}\big(A^T B\big),$$

where T denotes transpose in the chosen basis, show that

$$\langle\psi_0|(I_Q \otimes W_R)|\phi_0\rangle = \mathrm{Tr}\left(W^T \sqrt{\rho}\sqrt{\sigma}\right)$$

for any operator W_R on R.

iii) Deduce Uhlmann's theorem from (i), (ii), and part (b). Also conclude that $F(\rho,\sigma) = F(\sigma,\rho)$.

Solution: i) Since $\mathrm{Tr}_R(|\Omega\rangle\langle\Omega|) = I_Q$,

$$\mathrm{Tr}_R |\psi_0\rangle\langle\psi_0| = \sqrt{\rho}\ \mathrm{Tr}_R(|\Omega\rangle\langle\Omega|)\ \sqrt{\rho} = \rho,$$

and similarly $\mathrm{Tr}_R |\phi_0\rangle\langle\phi_0| = \sigma$. Thus $|\psi_0\rangle$ and $|\phi_0\rangle$ are purifications.

Now use the known fact that any two purifications of the same state are related by a unitary on the purifying system. Hence every purification of ρ has the form

$$|\psi\rangle = (I_Q \otimes U_R)|\psi_0\rangle$$

for some unitary U_R on R, and similarly every purification of σ has the form

$$|\phi\rangle = (I_Q \otimes V_R)|\phi_0\rangle.$$

This follows from the Schmidt decomposition because any purification of ρ has the same Schmidt coefficients as $|\psi_0\rangle$ on the Q side, so the only freedom is a unitary change of basis on R.

ii) Using the definitions,

$$\begin{aligned}\langle\psi_0|(I \otimes W)|\phi_0\rangle &= \langle\Omega|(\sqrt{\rho} \otimes I)(I \otimes W)(\sqrt{\sigma} \otimes I)|\Omega\rangle \\ &= \langle\Omega|(\sqrt{\rho}\sqrt{\sigma} \otimes W)|\Omega\rangle \\ &= \mathrm{Tr}\left((\sqrt{\rho}\sqrt{\sigma})^T W\right) = \mathrm{Tr}\left(W^T \sqrt{\rho}\sqrt{\sigma}\right).\end{aligned}$$

iii) Let

$$|\psi\rangle = (I \otimes U)|\psi_0\rangle, \qquad |\phi\rangle = (I \otimes V)|\phi_0\rangle.$$

Then

$$\langle\psi|\phi\rangle = \langle\psi_0|(I \otimes U^\dagger V)|\phi_0\rangle.$$

As $W = U^\dagger V$ ranges over all unitaries on R, part (ii) gives

$$\max_{|\psi\rangle,|\phi\rangle} |\langle\psi|\phi\rangle| = \max_W \left|\mathrm{Tr}\left(W^T \sqrt{\rho}\sqrt{\sigma}\right)\right|.$$

Since W^T is unitary whenever W is, the lemma from part (b) implies

$$\max_{|\psi\rangle,|\phi\rangle} |\langle\psi|\phi\rangle| = \mathrm{Tr}\,|\sqrt{\rho}\sqrt{\sigma}|.$$

Now let

$$A = \sqrt{\rho}\sqrt{\sigma}.$$

Then

$$|A| = \sqrt{A^\dagger A} = \sqrt{(\sqrt{\rho}\sqrt{\sigma})^\dagger(\sqrt{\rho}\sqrt{\sigma})} = \sqrt{\sqrt{\sigma}\,\rho\,\sqrt{\sigma}},$$

since $(\sqrt{\rho}\sqrt{\sigma})^\dagger = \sqrt{\sigma}\sqrt{\rho}$ and $\sqrt{\rho}\sqrt{\rho} = \rho$. Therefore

$$\max_{|\psi\rangle,|\phi\rangle} |\langle\psi|\phi\rangle| = \mathrm{Tr}\,|\sqrt{\rho}\sqrt{\sigma}| = \mathrm{Tr}\,\sqrt{\sqrt{\sigma}\,\rho\,\sqrt{\sigma}} = F(\sigma,\rho).$$

The left-hand side is symmetric in ρ and σ, since $|\langle\psi|\phi\rangle| = |\langle\phi|\psi\rangle|$. Exchanging ρ and σ therefore gives

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

as well. Hence $F(\rho,\sigma) = F(\sigma,\rho)$.

Problem 3: Monotonicity and Contractivity under Quantum Channels

A key property of physically meaningful distinguishability measures is that noise should never make quantum states more distinguishable. In this problem, you will prove that quantum channels decrease trace distance (contractivity) and do not decrease fidelity (monotonicity), and then verify both properties numerically.

a) Contractivity of trace distance.

Let $\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger$ be a trace-preserving quantum operation ($\sum_k M_k^\dagger M_k = I$). Use the POVM-element characterization from Problem 1(b) to prove that

$$D\big(\mathcal{E}(\rho),\,\mathcal{E}(\sigma)\big) \le D(\rho,\sigma).$$

Hint[2].

Solution: By Problem 1(b),

$$D\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) = \max_{0\le E\le I} \mathrm{Tr}\big(E(\mathcal{E}(\rho)-\mathcal{E}(\sigma))\big).$$

[2] Start from the characterization in Problem 1(b). For a POVM element E on the output space, define

$$\widetilde{E} = \sum_k M_k^\dagger E M_k.$$

Show that $\widetilde{E}$ is again a POVM element, i.e. $0 \le \widetilde{E} \le I$. For positivity, test $\widetilde{E}$ on an arbitrary vector $|\psi\rangle$.

So fix any POVM element E with $0 \le E \le I$. Then

$$\begin{aligned}\mathrm{Tr}\big(E(\mathcal{E}(\rho)-\mathcal{E}(\sigma))\big) &= \mathrm{Tr}\left(E\sum_k M_k(\rho-\sigma)M_k^\dagger\right)\\ &= \sum_k \mathrm{Tr}\big(EM_k(\rho-\sigma)M_k^\dagger\big)\\ &= \sum_k \mathrm{Tr}\big(M_k^\dagger EM_k(\rho-\sigma)\big)\\ &= \mathrm{Tr}\Big(\widetilde{E}(\rho-\sigma)\Big),\end{aligned}$$

where

$$\widetilde{E} \equiv \sum_k M_k^\dagger E M_k.$$

We now show that $\widetilde{E}$ is also a POVM element.

First, $\widetilde{E} \ge 0$. To see this, let $|\psi\rangle$ be any vector. Then

$$\langle\psi|M_k^\dagger E M_k\,|\psi\rangle = \langle M_k\psi|E\,|M_k\psi\rangle.$$

Since $E \ge 0$, the right-hand side is always non-negative. Therefore

$$\langle\psi|M_k^\dagger E M_k\,|\psi\rangle \ge 0 \qquad \text{for all } |\psi\rangle,$$

so each operator $M_k^\dagger E M_k$ is positive. A sum of positive operators is positive, hence

$$\widetilde{E} = \sum_k M_k^\dagger E M_k \ge 0.$$

Next, we show that $\widetilde{E} \le I$. Since $E \le I$, we have $I - E \ge 0$. Using the same idea as above, for any vector $|\psi\rangle$,

$$\langle\psi|M_k^\dagger(I-E)M_k\,|\psi\rangle = \langle M_k\psi|(I-E)\,|M_k\psi\rangle \ge 0.$$

So $M_k^\dagger(I-E)M_k \ge 0$, which is equivalent to

$$M_k^\dagger E M_k \le M_k^\dagger M_k.$$

Summing over k gives

$$\widetilde{E} = \sum_k M_k^\dagger E M_k \le \sum_k M_k^\dagger M_k = I.$$

Thus $0 \le \widetilde{E} \le I$, so $\widetilde{E}$ is indeed a valid POVM element.

Therefore, by Problem 1(b),

$$\mathrm{Tr}\Big(\widetilde{E}(\rho-\sigma)\Big) \le D(\rho,\sigma).$$

This holds for every POVM element E, so taking the maximum over all $0 \le E \le I$ gives

$$D\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) \le D(\rho,\sigma). \qquad \checkmark$$

b) Monotonicity of fidelity.

Prove that for any trace-preserving quantum operation $\mathcal{E}$,

$$F\big(\mathcal{E}(\rho),\,\mathcal{E}(\sigma)\big) \geq F(\rho,\sigma)$$

by using Uhlmann's theorem (Problem 2(c)) together with

$$\mathcal{E}(\tau) = \mathrm{Tr}_E\big(U(\tau \otimes |0\rangle\langle 0|_E)U^\dagger\big)$$

for some unitary U on $Q \otimes E$. Hint[3].

Solution: By Uhlmann's theorem, we can choose purifications $|\psi\rangle_{QR}$ of ρ and $|\phi\rangle_{QR}$ of σ such that

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

Now add the extra system E in the state $|0\rangle_E$, and define

$$|\psi'\rangle_{QER} \equiv (U_{QE}\otimes I_R)\big(|\psi\rangle_{QR}\otimes|0\rangle_E\big), \qquad |\phi'\rangle_{QER} \equiv (U_{QE}\otimes I_R)\big(|\phi\rangle_{QR}\otimes|0\rangle_E\big).$$

These are pure states on $Q \otimes E \otimes R$. We claim that they are purifications of $\mathcal{E}(\rho)$ and $\mathcal{E}(\sigma)$.

For $|\psi'\rangle$, we have

$$\begin{aligned}\mathrm{Tr}_{ER}\big(|\psi'\rangle\langle\psi'|\big) &= \mathrm{Tr}_E\Big(U_{QE}\Big(\mathrm{Tr}_R(|\psi\rangle\langle\psi|_{QR})\otimes|0\rangle\langle 0|_E\Big)U_{QE}^\dagger\Big)\\ &= \mathrm{Tr}_E\Big(U_{QE}\big(\rho\otimes|0\rangle\langle 0|_E\big)U_{QE}^\dagger\Big)\\ &= \mathcal{E}(\rho).\end{aligned}$$

So $|\psi'\rangle$ purifies $\mathcal{E}(\rho)$. In the same way, $|\phi'\rangle$ purifies $\mathcal{E}(\sigma)$.

The key point is that the overlap is unchanged, because $U_{QE}\otimes I_R$ is unitary:

$$\big|\langle\psi'|\phi'\rangle\big| = \big|\langle\psi|\phi\rangle\big|.$$

Now apply Uhlmann's theorem to the output states. Since fidelity is the maximum overlap over all purifications,

$$F\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) \geq \big|\langle\psi'|\phi'\rangle\big| = \big|\langle\psi|\phi\rangle\big| = F(\rho,\sigma).$$

Therefore

$$F\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) \geq F(\rho,\sigma). \qquad \checkmark$$

c) Numerical verification.

Consider the complete dephasing channel in the computational basis (equivalently, the phase-flip channel with probability $p = \frac{1}{2}$):

$$\mathcal{E}(\rho) = \tfrac{1}{2}(\rho + Z\rho Z).$$

Apply this channel to the two states from Problem 1(a):

$$\rho = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}, \qquad \sigma = |+\rangle\langle+| = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}.$$

[3] Take purifications $|\psi\rangle_{QR}$ of ρ and $|\phi\rangle_{QR}$ of σ. Add an extra system E in the state $|0\rangle_E$, apply $U_{QE}\otimes I_R$, and compare the overlap before and after.

Compute $D(\mathcal{E}(\rho),\mathcal{E}(\sigma))$ and $F(\mathcal{E}(\rho),\mathcal{E}(\sigma))$, and verify explicitly that

$$D(\mathcal{E}(\rho),\mathcal{E}(\sigma)) \le D(\rho,\sigma), \qquad F(\mathcal{E}(\rho),\mathcal{E}(\sigma)) \ge F(\rho,\sigma).$$

Solution: Since ρ is diagonal, $Z\rho Z = \rho$, so

$$\mathcal{E}(\rho) = \rho = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix}.$$

For $\sigma = |+\rangle\langle +|$, we have $Z|+\rangle = |-\rangle$, so

$$Z\sigma Z = |-\rangle\langle -|.$$

Therefore

$$\mathcal{E}(\sigma) = \frac{1}{2}\big(|+\rangle\langle +| + |-\rangle\langle -|\big) = \frac{1}{2}I = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

Hence

$$\mathcal{E}(\rho) - \mathcal{E}(\sigma) = \begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix} - \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \begin{pmatrix} 1/4 & 0 \\ 0 & -1/4 \end{pmatrix}.$$

Its eigenvalues are $\pm 1/4$, so

$$D\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) = \frac{1}{4} = 0.25.$$

For the fidelity, the two output states are diagonal in the same basis, so

$$F\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) = \sqrt{\frac{3}{4}\cdot\frac{1}{2}} + \sqrt{\frac{1}{4}\cdot\frac{1}{2}} = \frac{\sqrt{3}+1}{2\sqrt{2}} \approx 0.966.$$

For comparison, let us also compute the original trace distance. We have

$$\rho - \sigma = \begin{pmatrix} 1/4 & -1/2 \\ -1/2 & -1/4 \end{pmatrix},$$

whose eigenvalues are $\pm\sqrt{5}/4$. Therefore

$$D(\rho,\sigma) = \frac{\sqrt{5}}{4} \approx 0.559.$$

For the original fidelity, since $\sigma = |+\rangle\langle +|$ is pure,

$$F(\rho,\sigma) = \sqrt{\langle +|\rho|+\rangle} = \sqrt{\frac{1}{2}} = \frac{1}{\sqrt{2}} \approx 0.707.$$

So the inequalities are verified explicitly:

$$D\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) = \frac{1}{4} \le \frac{\sqrt{5}}{4} = D(\rho,\sigma),$$

and

$$F\big(\mathcal{E}(\rho),\mathcal{E}(\sigma)\big) = \frac{\sqrt{3}+1}{2\sqrt{2}} \ge \frac{1}{\sqrt{2}} = F(\rho,\sigma).$$

The channel removes the off-diagonal coherence in σ, so the two output states are less distinguishable: the trace distance goes down, and the fidelity goes up. ✓

Problem 4: Relating Trace Distance and Fidelity

The trace distance and fidelity are two different ways to quantify how distinguishable two quantum states are. The standard relation between them is given by the *Fuchs–van de Graaf inequalities*:

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

In this problem you will prove the *upper bound*

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

and show that it is tight for pure states. The lower bound

$$1 - F(\rho,\sigma) \;\le\; D(\rho,\sigma)$$

is stated here without proof.

a) Pure states.

For pure states $|a\rangle$ and $|b\rangle$, show that

$$D(|a\rangle,|b\rangle) = \sqrt{1-F(|a\rangle,|b\rangle)^2}.$$

Solution: Both D and F are invariant under applying the same unitary to both states, so we may choose an orthonormal basis for the span of $|a\rangle$ and $|b\rangle$ such that

$$|a\rangle = |0\rangle, \qquad |b\rangle = \cos\theta\,|0\rangle + e^{i\phi}\sin\theta\,|1\rangle, \qquad 0 \le \theta \le \frac{\pi}{2}.$$

Then

$$F(|a\rangle,|b\rangle) = |\langle a|b\rangle| = \cos\theta.$$

The density matrices are $\rho_a = |0\rangle\langle 0|$ and

$$\rho_b = |b\rangle\langle b| = \begin{pmatrix} \cos^2\theta & e^{-i\phi}\cos\theta\sin\theta \\ e^{i\phi}\cos\theta\sin\theta & \sin^2\theta \end{pmatrix}.$$

Their difference is

$$\rho_a - \rho_b = \begin{pmatrix} \sin^2\theta & -e^{-i\phi}\cos\theta\sin\theta \\ -e^{i\phi}\cos\theta\sin\theta & -\sin^2\theta \end{pmatrix}.$$

This matrix is Hermitian and traceless, so its eigenvalues are $\pm\lambda$. Since

$$\det(\rho_a - \rho_b) = -\lambda^2 = -\sin^4\theta - \cos^2\theta\sin^2\theta = -\sin^2\theta,$$

we get $\lambda = \sin\theta$.

Therefore,

$$D(|a\rangle,|b\rangle) = \tfrac{1}{2}\operatorname{Tr}|\rho_a - \rho_b| = \tfrac{1}{2}\big(|\lambda| + |-\lambda|\big) = \sin\theta = \sqrt{1-\cos^2\theta} = \sqrt{1-F(|a\rangle,|b\rangle)^2}. \qquad \checkmark$$

b) Upper bound: $D(\rho,\sigma) \le \sqrt{1-F(\rho,\sigma)^2}$**.**

i) Let X be a Hermitian operator on $Q \otimes R$. Show that

$$\operatorname{Tr}\big|\operatorname{Tr}_R(X)\big| \le \operatorname{Tr}|X|.$$

ii) Use part (i), together with Uhlmann's theorem and part (a), to prove that

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

for arbitrary density operators ρ and σ.

Solution: i) Write spectral decompositions

$$X = \sum_i x_i \,|i\rangle\langle i|, \qquad \mathrm{Tr}_R(X) = \sum_j y_j \,|u_j\rangle\langle u_j|,$$

with $x_i, y_j \in \mathbb{R}$. Then

$$y_j = \langle u_j|\,\mathrm{Tr}_R(X)\,|u_j\rangle = \sum_i x_i \,\langle u_j|\,\mathrm{Tr}_R(|i\rangle\langle i|)\,|u_j\rangle.$$

Define

$$a_{ij} := \langle u_j|\,\mathrm{Tr}_R(|i\rangle\langle i|)\,|u_j\rangle.$$

Each operator $\mathrm{Tr}_R(|i\rangle\langle i|)$ is positive and has trace 1, so

$$a_{ij} \geq 0, \qquad \sum_j a_{ij} = \mathrm{Tr}\big(\mathrm{Tr}_R(|i\rangle\langle i|)\big) = 1.$$

Hence

$$|y_j| \leq \sum_i |x_i|\, a_{ij}.$$

Summing over j gives

$$\mathrm{Tr}\big|\mathrm{Tr}_R(X)\big| = \sum_j |y_j| \leq \sum_i |x_i| \sum_j a_{ij} = \sum_i |x_i| = \mathrm{Tr}\,|X|.$$

ii) By Uhlmann's theorem (Problem 2c), there exist purifications $|\psi\rangle$ of ρ and $|\phi\rangle$ of σ on some larger space $Q \otimes R$ such that

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

Let

$$\Delta = |\psi\rangle\langle\psi| - |\phi\rangle\langle\phi|.$$

Then Δ is Hermitian and

$$\rho - \sigma = \mathrm{Tr}_R(\Delta).$$

Applying part (i) with $X = \Delta$,

$$\mathrm{Tr}\,|\rho-\sigma| = \mathrm{Tr}\big|\mathrm{Tr}_R(\Delta)\big| \leq \mathrm{Tr}\,|\Delta|.$$

Therefore

$$D(\rho,\sigma) = \tfrac{1}{2}\,\mathrm{Tr}\,|\rho-\sigma| \leq \tfrac{1}{2}\,\mathrm{Tr}\,|\Delta| = D(|\psi\rangle,|\phi\rangle).$$

By part (a),

$$D(|\psi\rangle,|\phi\rangle) = \sqrt{1-|\langle\psi|\phi\rangle|^2} = \sqrt{1-F(\rho,\sigma)^2}.$$

Hence

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