

Quantum information theory

Lectures 10-14

Quantum states: II-VI. Multiple systems and entanglement.

Gleason's theorem. For $D \geq 3$, if a function f from 1-d projectors to $[0,1]$ satisfies $\sum_j f(P_j) = 1$, whenever $\sum_j P_j = 1$, then there exists a density operator ρ such that $f(P) = \text{tr}(\rho P)$.

Axiomatization of gm. State space from Hilbert-space structure of quantum measurements.

Why Hilbert space?

Why noncontextual probabilities?

Partial trace and marginal density operators (See additional notes)

Operator $O = \sum_{j,k,l,m} |e_j, f_k\rangle \langle e_l, f_m| O_{j,k,l,m}$

Partial trace:

$$\text{tr}_B(O) = \sum_k \underbrace{\langle f_k | O | f_k \rangle}_{\text{operator on A}} = \sum_{j,l} |e_j\rangle \langle e_l| \sum_k O_{j,k,l,k}$$

Measure in basis $|e_j\rangle$ on A:

$$P(e_j) = \sum_k P(e_j, f_k) = \sum_k \langle e_j, f_k | \rho | e_j, f_k \rangle = \langle e_j | \sum_k \langle f_k | \rho | f_k \rangle | e_j \rangle$$

$$= \text{tr}_B(\rho) = \rho_A = \left(\begin{array}{l} \text{marginal or} \\ \text{reduced density} \\ \text{operator of A} \end{array} \right)$$

$$= \text{tr} \left(\rho \underbrace{|e_j\rangle\langle e_j|}_{P_j} \otimes \underbrace{\sum_k |f_k\rangle\langle f_k|}_{I_B} \right) = \text{tr} \left(\rho P_j \otimes I_B \right) \quad \textcircled{3}$$

↓
projection operator
for a measurement
on A

$$= \text{tr} \left(\rho_A P_j \right)$$

Two qubits

Orthonormal basis: $|00\rangle = |0\rangle \otimes |0\rangle$
 (standard) $|01\rangle = |0\rangle \otimes |1\rangle$
 $|10\rangle = |1\rangle \otimes |0\rangle$
 $|11\rangle = |1\rangle \otimes |1\rangle$

} $|x\rangle = |x_1\rangle \otimes |x_2\rangle$

Bell (orthonormal) basis:

$Z \otimes Z, X \otimes X, Y \otimes Y$ commute

$$\begin{cases} |\Phi^\pm\rangle = \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle) = \begin{matrix} |\beta_{00}\rangle \\ |\beta_{10}\rangle \end{matrix} \\ |\Psi^\pm\rangle = \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle) = \begin{matrix} |\beta_{01}\rangle \\ |\beta_{11}\rangle \end{matrix} \end{cases}$$

$$\begin{aligned} Z \otimes Z |\Phi^\pm\rangle &= |\Phi^\pm\rangle && \text{"parity" bit} \\ Z \otimes Z |\Psi^\pm\rangle &= -|\Psi^\pm\rangle && \Phi \text{ vs. } \Psi \\ X \otimes X |\Phi^\pm\rangle &= \pm |\Phi^\pm\rangle && \text{"phase" bit} \\ X \otimes X |\Psi^\pm\rangle &= \pm |\Psi^\pm\rangle && \pm \text{ vs. } - \end{aligned}$$

Singlet vs. triplet

$$|\beta_{ab}\rangle = \frac{1}{\sqrt{2}} (|0b\rangle + (-1)^a |1\bar{b}\rangle)$$

phase bit \uparrow parity bit \leftarrow \leftarrow $1 \otimes b$

$$\begin{aligned} Z \otimes Z |\beta_{ab}\rangle &= (-1)^b |\beta_{ab}\rangle \\ X \otimes X |\beta_{ab}\rangle &= (-1)^a |\beta_{ab}\rangle \end{aligned}$$

Marginal density operators: $\rho_A = \rho_B = \frac{1}{2} I$

Entangled: $|\Phi\rangle = \underbrace{|1/\sqrt{2}\rangle \otimes |1/\sqrt{2}\rangle}_{\text{product pure state}}$

Generally, we can write the Pauli representations as

$$|\beta_{ab}\rangle\langle\beta_{ab}| = \frac{1}{4} (1 \otimes 1 + (-1)^b Z \otimes Z + (-1)^a X \otimes X - (-1)^{a+b} Y \otimes Y)$$

These are the eigenvalues below

Inverting these relations, we find

$$\begin{aligned} 1 \otimes 1 &= +|\beta_{00}\rangle\langle\beta_{00}| + |\beta_{10}\rangle\langle\beta_{10}| + |\beta_{01}\rangle\langle\beta_{01}| + |\beta_{11}\rangle\langle\beta_{11}| \\ Z \otimes Z &= +|\beta_{00}\rangle\langle\beta_{00}| + |\beta_{10}\rangle\langle\beta_{10}| - |\beta_{01}\rangle\langle\beta_{01}| - |\beta_{11}\rangle\langle\beta_{11}| \\ X \otimes X &= +|\beta_{00}\rangle\langle\beta_{00}| - |\beta_{10}\rangle\langle\beta_{10}| + |\beta_{01}\rangle\langle\beta_{01}| - |\beta_{11}\rangle\langle\beta_{11}| \\ Y \otimes Y &= -|\beta_{00}\rangle\langle\beta_{00}| + |\beta_{10}\rangle\langle\beta_{10}| + |\beta_{01}\rangle\langle\beta_{01}| - |\beta_{11}\rangle\langle\beta_{11}| \end{aligned}$$



These are commuting operators
Any two of $X \otimes X$, $Y \otimes Y$, and $Z \otimes Z$ is a complete set of commuting operators



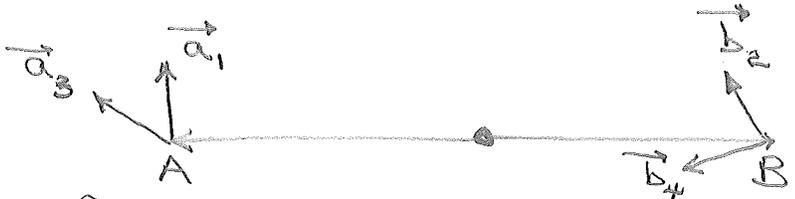
These are the simultaneous eigendecompositions in terms of Bell states.

$Z \otimes Z |\beta_{ab}\rangle = (-1)^b |\beta_{ab}\rangle$; a measurement of $Z \otimes Z$ determines the parity bit.

$X \otimes X |\beta_{ab}\rangle = (-1)^a |\beta_{ab}\rangle$; a measurement of $X \otimes X$ determines the phase bit.

$$\begin{aligned} Y \otimes Y |\beta_{ab}\rangle &= -(-1)^{a+b} |\beta_{ab}\rangle \\ \implies Z \otimes X \otimes Z \otimes X &= -X \otimes Z \otimes X \otimes Z \end{aligned}$$

CHSH Bell inequality:



Realism: Values of $\sigma_a, \sigma_b = \pm 1$ are objective properties of A and B.

No-disturbance: Measurement on A does not disturb objective values of B

↑
enforced by locality

Local realism

$C(\vec{a}, \vec{b}) = \langle \sigma_a \sigma_b \rangle = a_i b_j \langle \sigma_i \sigma_j \rangle = -a_i b_j$

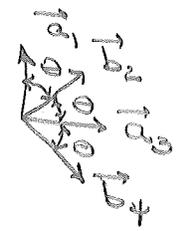
$$|\sigma_{a_1}(\sigma_{b_2} - \sigma_{b_3}) + \sigma_{a_2}(\sigma_{b_2} + \sigma_{b_3})| = 2$$

$$\langle \sigma_{a_1} \sigma_{b_2} - \sigma_{a_1} \sigma_{b_3} + \sigma_{a_2} \sigma_{b_2} + \sigma_{a_2} \sigma_{b_3} \rangle = 2$$

$$|\underbrace{\langle \sigma_{a_1} \sigma_{b_2} \rangle + \langle \sigma_{a_2} \sigma_{b_2} \rangle + \langle \sigma_{a_2} \sigma_{b_3} \rangle - \langle \sigma_{a_1} \sigma_{b_3} \rangle}_{= 5}| \leq 2$$

CHSH Bell inequality

QM: $|\Psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ singlet: rotationally invariant



$$C(\vec{a}, \vec{b}) = \langle \sigma_a \sigma_b \rangle = -\vec{a} \cdot \vec{b} = -\cos\theta_{ab}$$

$$\Rightarrow S = |3\cos\theta - \cos 3\theta| \rightarrow 2\sqrt{2} \text{ for } \theta = 45^\circ$$

For $\theta = 45^\circ$, $\vec{a}_1 = \vec{e}_z$, $\vec{b}_2 = \frac{1}{\sqrt{2}}(\vec{e}_y + \vec{e}_x)$, $\vec{a}_2 = \vec{e}_y$, $\vec{b}_3 = \frac{1}{\sqrt{2}}(\vec{e}_y - \vec{e}_x)$

$$S = \langle X \otimes \frac{1}{\sqrt{2}}(Y+X) + Y \otimes \frac{1}{\sqrt{2}}(Y+X) + Y \otimes \frac{1}{\sqrt{2}}(Y-X) - X \otimes \frac{1}{\sqrt{2}}(Y-X) \rangle$$

$$= \sqrt{2} \langle X \otimes X + Y \otimes Y \rangle$$

$$= 2\sqrt{2} \langle |\beta_{01}\rangle \langle \beta_{01}| - |\beta_{11}\rangle \langle \beta_{11}| \rangle$$

Maximal violation for $|\beta_{01}\rangle$ (correlations) or $|\beta_{11}\rangle$ (anticorrelations)

Teleportation: Alice and Bob each has one of a pair of qubits in entangled state $|\beta_{00}^{AB}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Victor hands to Alice a qubit in state $|\psi^A\rangle$.

Total state: $|\Psi\rangle = |\psi^A\rangle \otimes |\beta_{00}^{AB}\rangle$

$$= \sum_{a,b} |\beta_{ab}^{VA}\rangle \langle \beta_{ab}^{VA} | \Psi \rangle$$

vector in Bob's Hilbert space magnitude times "relative state"

$$\langle \beta_{00}^{VA} | \Psi \rangle = \langle \beta_{00}^{VA} | (|\psi^A\rangle \otimes |\beta_{00}^{AB}\rangle)$$

$$= \frac{1}{\sqrt{2}} (\langle 00 | + \langle 11 |) (|\psi^A\rangle \otimes (|00\rangle + |11\rangle))$$

$$= \frac{1}{\sqrt{2}} (\langle 0 | \psi^A \rangle |0\rangle + \langle 1 | \psi^A \rangle |1\rangle)$$

$$= \frac{1}{\sqrt{2}} |\psi^B\rangle$$

relative state in B
 $|\psi\rangle$ belonging to B

compare

$$\langle \beta_{ab}^{VA} | \Psi \rangle = (\langle \beta_{00}^{VA} | X^b Z^a \otimes 1 (|\psi^A\rangle \otimes |\beta_{00}^{AB}\rangle)$$

$$= \langle \beta_{00}^{VA} | (X^b Z^a |\psi^A\rangle \otimes |\beta_{00}^{AB}\rangle)$$

$$= \frac{1}{\sqrt{2}} X^b Z^a |\psi^B\rangle \quad \text{relative state in B}$$

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \sum_{a,b} |\beta_{ab}^{VA}\rangle \otimes X^b Z^a |\psi^B\rangle$$

$$= \frac{1}{\sqrt{2}} (|\beta_{00}^{VA}\rangle \otimes |\psi^B\rangle + |\beta_{01}^{VA}\rangle \otimes X|\psi^B\rangle + |\beta_{10}^{VA}\rangle \otimes Z|\psi^B\rangle + |\beta_{11}^{VA}\rangle \otimes XZ|\psi^B\rangle)$$

Alice measures in the Bell basis (all 4 results equally likely; no trace of $|\psi^A\rangle$ left in VA), sends 2 bits, a and b , to Bob, who applies the appropriate unitary, $Z^a X^b$, to leave his qubit in state $|\psi^A\rangle$.

Non-square matrices: add rows and columns of zeros to make matrix square.

Polar decomposition and singular values. Given any

operator A , $A^\dagger A$ and AA^\dagger are positive operators with the same (nonnegative) eigenvalues, whose square roots are the singular values of A .

Moreover, there exists a unitary operator U such that

$$A = U\sqrt{A^\dagger A} = \sqrt{AA^\dagger}U \quad \leftarrow \text{polar decomposition}$$

U is unique if $A^\dagger A$ is invertible. The eigenvectors $|e_j\rangle$ of $A^\dagger A$ are called the right singular vectors of A , and the eigenvectors $|f_j\rangle$ of AA^\dagger are called the left singular vectors of A .

$A \text{ is normal} \iff [U, A^\dagger A] = 0$

Proof:

Eigendecomposition $A^\dagger A = \sum_j \lambda_j^2 |e_j\rangle\langle e_j|$, $A^\dagger A |e_j\rangle = \lambda_j^2 |e_j\rangle$.

Let $S_{A^\dagger A}$ be the support of $A^\dagger A$, and let $N_{A^\dagger A}$ be the null subspace. Now

$$AA^\dagger(A|e_j\rangle) = A(A^\dagger A|e_j\rangle) = \lambda_j^2 A|e_j\rangle$$

$\Rightarrow A|e_j\rangle$ is an eigenvector of AA^\dagger with eigenvalue λ_j^2 .

Two cases:

(i) $\lambda_j = 0$ ($|e_j\rangle \in N_{A^\dagger A}$): $\langle e_j | A^\dagger A | e_j \rangle = 0 \Rightarrow A|e_j\rangle = 0$

(ii) $\lambda_j \neq 0$ ($|e_j\rangle \in S_{A^\dagger A}$): Define $|f_j\rangle \equiv \frac{A|e_j\rangle}{\langle e_j | A^\dagger A | e_j \rangle^{1/2}} = A|e_j\rangle / \lambda_j$.

Notice that $\langle f_j | f_k \rangle = \langle e_j | A^\dagger A | e_k \rangle / \lambda_j \lambda_k = \delta_{jk}$, so the vectors $|f_j\rangle$ are orthonormal eigenvectors of AA^\dagger .

Now

$$\begin{aligned}
 (AA^T)^2 &= A(A^T A)A^T = \sum_j \lambda_j^2 A|e_j\rangle\langle e_j|A^T \\
 &= \sum_{\lambda_j \neq 0} \lambda_j^2 \underbrace{A|e_j\rangle\langle e_j|A^T}_{\lambda_j^2 |f_j\rangle\langle f_j|} \\
 &= \sum_{\lambda_j \neq 0} \lambda_j^2 |f_j\rangle\langle f_j|
 \end{aligned}$$

eigendecomposition of $(AA^T)^2$

$$\Rightarrow AA^T = \underbrace{\sum_{\lambda_j \neq 0} \lambda_j^2 |f_j\rangle\langle f_j|}_{\text{eigendecomposition of } AA^T} \Rightarrow \begin{array}{l} \text{The vectors } |f_j\rangle \text{ span} \\ \text{the support } S_{AA^T}. \end{array}$$

Now complete the orthonormal basis $|f_j\rangle$ by adding on any orthonormal vectors in the null subspace of AA^T . For all j , we can write

$$A|e_j\rangle = \lambda_j |f_j\rangle = \begin{cases} \lambda_j |f_j\rangle, & \lambda_j \neq 0 \\ 0, & \lambda_j = 0 \end{cases}$$

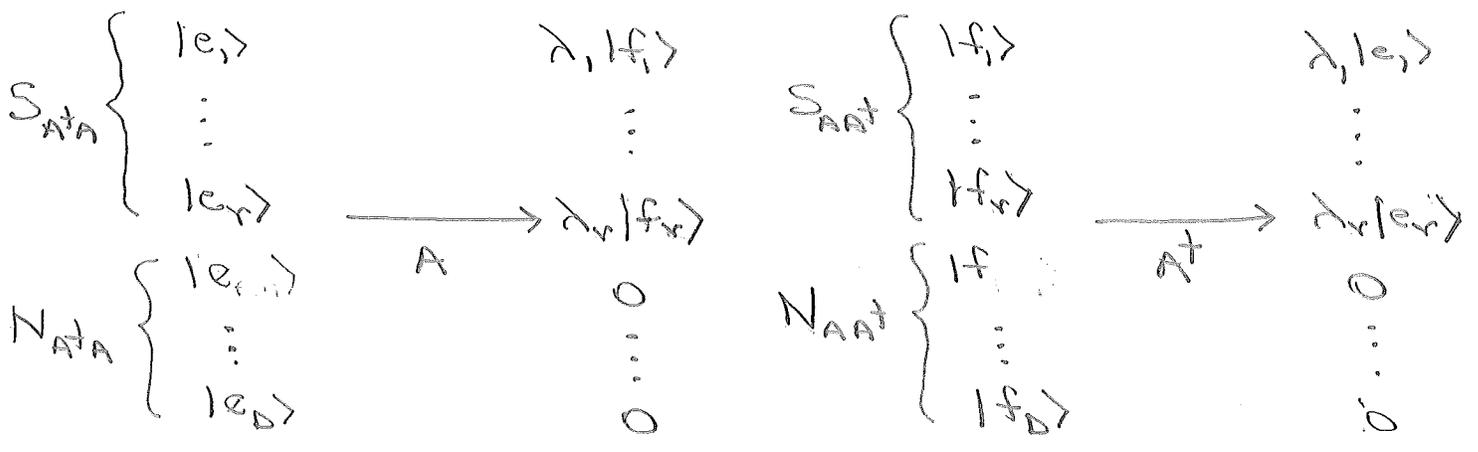
Thus A has the form

$$A = \sum_{j,k} |f_j\rangle\langle f_j| \underbrace{A|e_k\rangle\langle e_k|}_{\lambda_j \langle f_j|f_k\rangle = \lambda_j \delta_{jk}} \langle e_k| = \sum_j \lambda_j |f_j\rangle\langle e_j|$$

↑
right singular vectors
left singular vectors

Summary till now:

$$\begin{aligned}
 A &= \sum_j \lambda_j |f_j\rangle\langle e_j| & A^T A &= \sum_j \lambda_j^2 |e_j\rangle\langle e_j| \\
 A^T &= \sum_j \lambda_j |e_j\rangle\langle f_j| & AA^T &= \sum_j \lambda_j^2 |f_j\rangle\langle f_j|
 \end{aligned}$$



r is the rank of A

Finishing off, we can define the unitary operator $U = \sum_j |f_j\rangle \langle e_j|$, i.e., $U|e_j\rangle = |f_j\rangle$ (unitary because U maps orthonormal basis $|e_j\rangle$ to orthonormal basis $|f_j\rangle$). Thus

$$\begin{aligned}
 A &= \sum_j \lambda_j |f_j\rangle \langle e_j| \\
 &= \left(\sum_j |f_j\rangle \langle e_j| \right) \sqrt{A^t A} = U \sqrt{A^t A} \\
 &= \sqrt{A A^t} \left(\sum_j |f_j\rangle \langle e_j| \right) = \sqrt{A A^t} U
 \end{aligned}$$

The freedom in U is the freedom in how it maps $N_{A^t A}$ to N_{AA^t} . There is no freedom if $A^t A$ has no zero eigenvalues, for then $A^t A$ is invertible and

$$U = A \underbrace{(A^t A)^{-1/2}}_{(\sqrt{A^t A})^{-1}}$$

Going from $A^t A$ to A :

$$\begin{aligned}
 A &= \sqrt{A^t A} U \\
 A &= \sqrt{A^t A} \uparrow \uparrow \sqrt{A A^t} \\
 &\uparrow \uparrow
 \end{aligned}$$

Singular-value decomposition.

Given an operator A and an arbitrary orthonormal basis $|g_j\rangle$, there exist unitary operators V and W such that $A = V \Lambda W^\dagger$, where

$$\Lambda = \sum_j \lambda_j |g_j\rangle \langle g_j|$$

$$A = \sum_j \lambda_j \underbrace{V|g_j\rangle}_{|f_j\rangle} \underbrace{\langle g_j|W^\dagger}_{\langle e_j|}$$

is diagonal in the basis $|g_j\rangle$, its eigenvalues being the singular values of A .

Proof:

$$A = U \sqrt{A^\dagger A} = U \underbrace{\sum_j \lambda_j |e_j\rangle \langle e_j|}_{\text{eigendecomposition of } \sqrt{A^\dagger A}} = \underbrace{U W}_{\equiv V} \left(\sum_j \lambda_j |g_j\rangle \langle g_j| \right) \underbrace{W^\dagger}_{\equiv \Lambda}$$

\uparrow
 polar decomposition

Unitary W defined by $W|g_j\rangle = |e_j\rangle$
 Notice that $V|g_j\rangle = |f_j\rangle$

Relative states.

$|\phi_\alpha\rangle = \sqrt{p_\alpha} |\psi_\alpha\rangle$ is a vector in \mathcal{H}_A

Bipartite pure state

$$|\Psi\rangle = \sum_\alpha |f_\alpha\rangle \langle f_\alpha | \Psi \rangle = \sum_\alpha \sqrt{p_\alpha} |\psi_\alpha\rangle \otimes |f_\alpha\rangle$$

\uparrow
 orthonormal basis for B

\uparrow
 relative state

$$\rho_A = \text{tr}_B (|\Psi\rangle \langle \Psi|) = \sum_{\alpha, \beta} \sqrt{p_\alpha p_\beta} |\psi_\alpha\rangle \langle \psi_\beta| \text{tr} (|f_\alpha\rangle \langle f_\beta|)$$

$$\sum_{\alpha, \beta} \sqrt{p_\alpha p_\beta} |\psi_\alpha\rangle \langle \psi_\beta| \otimes |f_\alpha\rangle \langle f_\beta| \quad \langle f_\beta | f_\alpha \rangle = \delta_{\alpha\beta}$$

$$\rho_A = \sum_\alpha p_\alpha |\psi_\alpha\rangle \langle \psi_\alpha| \leftarrow \begin{array}{l} \text{ensemble decomposition} \\ \text{of } \rho_A \end{array}$$

\uparrow
 not necessarily orthonormal

Schmidt decomposition. Any bipartite pure state

can be written as

$$|\Psi\rangle = \sum_j \sqrt{\lambda_j} |e_j\rangle \otimes |f_j\rangle.$$

special relative-state decomposition

orthonormal vectors in \mathcal{H}_B

orthonormal vectors in \mathcal{H}_A

nonnegative Schmidt coefficients

Schmidt vectors

As a consequence, $\rho_A = \sum_j \lambda_j |e_j\rangle\langle e_j|$ and $\rho_B = \sum_j \lambda_j |f_j\rangle\langle f_j|$ have the same eigenvalues.

What's the point? Schmidt coefficients provide a complete characterization of bipartite pure-state entanglement. Schmidt coefficients are invariant under local unitaries. Schmidt vectors can be mapped to any pair of bases by local unitaries. There is no Schmidt-like decomposition for 3 or more systems.

Proof: Diagonalize $\rho_B = \text{tr}_A(|\Psi\rangle\langle\Psi|) = \sum_j \lambda_j |f_j\rangle\langle f_j|$.

Form the relative-state decomposition wrt to the vectors $|f_j\rangle$, $|\Psi\rangle = \sum_j |e_j\rangle \otimes |f_j\rangle$, and calculate ρ_B explicitly,

$$\rho_B = \text{tr}_A(|\Psi\rangle\langle\Psi|) = \sum_{j,k} \text{tr}(|e_j\rangle\langle e_k|) |f_j\rangle\langle f_k|$$

$$= \sum_{j,k} |e_j\rangle\langle e_k| \otimes |f_j\rangle\langle f_k| \quad \langle e_j | e_k \rangle$$

$$\rho_B = \sum_{j,k} \langle e_j | e_k \rangle |f_j\rangle\langle f_k| \Rightarrow \langle e_j | e_k \rangle = \lambda_j \delta_{jk}$$

Introducing orthonormal vectors $|e_j\rangle = |e_j\rangle / \sqrt{\lambda_j}$ for $\lambda_j \neq 0$, we have

$$|\Psi\rangle = \sum_j \sqrt{\lambda_j} |e_j\rangle \otimes |f_j\rangle.$$

Purifications. $|\Psi\rangle$ is a purification of ρ_A if

$$\rho_A = \text{tr}_B(|\Psi\rangle\langle\Psi|).$$

What's the point?

- ① ρ_A can arise from an entangled bipartite pure state
- ② A purification can be a useful analytical tool, replacing a mixed-state analysis with a pure-state analysis on a larger space

THE CHURCH OF THE LARGER HILBERT SPACE

Ensemble decomposition

$$\rho_A = \sum_{\alpha} p_{\alpha} |\psi_{\alpha}\rangle\langle\psi_{\alpha}|$$

Purification

$$|\Psi\rangle = \sum_{\alpha} \sqrt{p_{\alpha}} |\psi_{\alpha}\rangle \otimes |\phi_{\alpha}\rangle$$

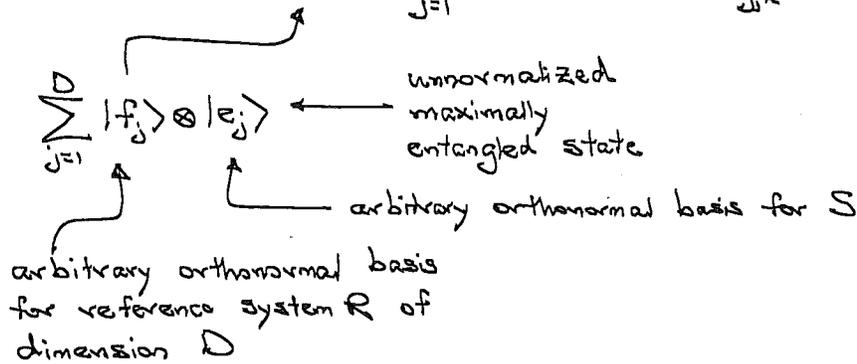
↑
relative-state decomposition

↑
orthonormal vectors in \mathcal{H}_B

Putting it all together: purifications, ensemble decompositions, relative states, and Neumark extensions

VEC'ing an operator: VEC maps operator A on system S to a vector

$$|A\rangle = |\mathbb{I}_A\rangle \equiv \mathbb{1} \otimes A |\mathbb{I}\rangle = \sum_{j=1}^D |f_j\rangle \otimes A|e_j\rangle = \sum_{j,k} |f_j\rangle \otimes |e_k\rangle \underbrace{\langle e_k | A | e_j \rangle}_{A_{kj}}$$



Recover A from $|A\rangle$ via $\langle f_j, e_k | A \rangle = A_{kj}$ VEC is 1-1 and onto

$$|A\rangle\langle B| = \sum_{j,k} |f_j\rangle\langle f_k| \otimes A|e_j\rangle\langle e_k| B^\dagger$$

VEC preserves inner products: $\langle A|B\rangle = \text{tr}(A^\dagger B)$

$$\text{tr}_R(|A\rangle\langle A|) = \sum_j A|e_j\rangle\langle e_j| A^\dagger = AA^\dagger \leftarrow |A\rangle \text{ is a "purification" of } AA^\dagger$$

$$\text{tr}_S(|A\rangle\langle A|) = \sum_{j,k} |f_j\rangle\langle f_k| \langle e_k | A^\dagger A | e_j \rangle = (A^\dagger A)^\top \uparrow \text{ in } R$$

in fiducial basis $|f_j\rangle$

Note: $|A\rangle = \mathbb{1} \otimes A |\mathbb{I}\rangle = \sum_{j,k} |f_j\rangle \otimes |e_k\rangle \langle e_k | A | e_j \rangle$

$$= \sum_{j,k} |f_j\rangle\langle f_j| A^\dagger |f_k\rangle \otimes |e_k\rangle = A^\dagger \otimes \mathbb{1} |\mathbb{I}_{f_k}\rangle$$

Note: SVD of $A_{kj} = (V \Lambda W^\dagger)_{kj}$ gives Schmidt decomposition of $|A\rangle$.
 (choose diagonal in $|e_j\rangle$)

$$|A\rangle = \sum_{j,k} |f_j\rangle \otimes \underbrace{V \Lambda W^\dagger |e_j\rangle}_{\lambda_j V |e_j\rangle = \lambda_j |f_j\rangle} = \sum_j \lambda_j |f_j\rangle \otimes |f_j\rangle$$

Consider a positive operator $G = \sum_j \lambda_j |g_j\rangle\langle g_j|$ (G is a density operator if $\text{tr}(G) = 1$).

$$\begin{aligned}
 |\sqrt{G}\rangle &= |\mathbb{1}\sqrt{G}\rangle = \mathbb{1} \otimes \sqrt{G} |\mathbb{1}\rangle = \sum_{j=1}^{\text{rank of } G} |f_j\rangle \otimes \sqrt{\lambda_j} |g_j\rangle = \sum_{j=1}^r \sqrt{\lambda_j} |f_j\rangle \otimes |g_j\rangle \\
 &= \sum_{j=1}^r |f_j\rangle \otimes |g_j\rangle
 \end{aligned}$$

\uparrow "fiducial purification" of G

Extend \mathcal{R} to arbitrary dimension N . By the Schmidt decomposition, any two "purifications" of G differ only by the orthogonal Schmidt vectors in \mathcal{R} and thus are related by a unitary in \mathcal{R} .

$$\begin{aligned}
 |\mathbb{1}\rangle &= U \otimes \mathbb{1} |\sqrt{G}\rangle = \sum_{j=1}^r U |f_j\rangle \otimes \sqrt{\lambda_j} |g_j\rangle \\
 &= \sum_{j=1}^r \sum_{\alpha=1}^N |f_\alpha\rangle \langle f_\alpha| U |f_j\rangle \otimes \sqrt{\lambda_j} |g_j\rangle \\
 &= \sum_{\alpha=1}^N |f_\alpha\rangle \otimes \sqrt{\lambda_j} \sum_{j=1}^r U_{\alpha j} |g_j\rangle \\
 &= \sqrt{\lambda_j} \sum_{\beta=1}^N |g_\beta\rangle \langle g_\beta| U_{\alpha j} |g_j\rangle \quad \left\{ \begin{array}{l} \text{Track on additional} \\ \text{basis states in } S \end{array} \right. \\
 &\quad \left\{ \begin{array}{l} \text{Extend } U_{\alpha j} \text{ to an} \\ \text{N} \times \text{N unitary matrix} \\ U_{\alpha\beta} \end{array} \right. \quad (\sqrt{\lambda_j} |g_\beta\rangle = 0 \text{ for } \beta > r) \\
 &= \sqrt{\lambda_j} \sum_{\beta=1}^N |g_\beta\rangle \langle g_\beta| U^T |e_\alpha\rangle \\
 &= \sqrt{\lambda_j} U^T |g_\alpha\rangle \\
 &= \mathbb{1} \otimes \sqrt{\lambda_j} U^T \sum_{\alpha=1}^N |f_\alpha\rangle \otimes |g_\alpha\rangle \\
 &\quad \underbrace{\sum_{\alpha=1}^N |f_\alpha\rangle}_{|\tilde{\mathbb{1}}\rangle}
 \end{aligned}$$

We end up with several ways to write an arbitrary purification of G :

↙ arbitrariness is in U

$$|\Phi\rangle = U \otimes 1 |\sqrt{G}\rangle = U \otimes \sqrt{G} |\Psi\rangle$$

$$= 1 \otimes \sqrt{G} U^T |\Psi\rangle$$

relative-state decomposition

$$= \sum_{\alpha=1}^N |f_{\alpha}\rangle \otimes |\bar{f}_{\alpha}\rangle$$

$$|\bar{f}_{\alpha}\rangle = \sqrt{G} U^T |g_{\alpha}\rangle = \sum_{j=1}^r U_{\alpha j} \sqrt{G} |g_j\rangle = \sum_{j=1}^r U_{\alpha j} \sqrt{\lambda_j} |g_j\rangle$$

are a decomposition of G .

Purifications and ensemble decompositions are in 1-1 correspondence, both specified by $N \times r$ partial unitary matrix $U_{\alpha j}$.

HJW theorem

$$= \sum_{\alpha=1}^N |f_{\alpha}\rangle \otimes \sqrt{G} |\bar{f}_{\alpha}\rangle$$

$|\bar{f}_{\alpha}\rangle = \sum_{j=1}^r U_{\alpha j} |g_j\rangle$ resolve the support of G (projector $P_G = \sum_{j=1}^r |g_j\rangle \langle g_j|$)

$$= \sum_{\alpha=1}^N |f_{\alpha}\rangle \otimes \sqrt{G} U^T |g_{\alpha}\rangle$$

orthonormal vectors in an extended space; called the Newmark extension of $|\bar{f}_{\alpha}\rangle$

$$P_G U^T |g_{\alpha}\rangle = \sum_j |g_j\rangle U_{\alpha j} = |\bar{f}_{\alpha}\rangle$$

The unitary matrix in a change between ensemble decompositions finds another home as a unitary operator U on \mathbb{R} , which transforms between purifications, or as a unitary operator U^T on S , which acts in the Newmark extension.