Partial traces and Purification

$(\rho_1 \otimes \rho_2) \otimes \rho_3$ $\qquad e^{i\theta}|\psi\rangle$

Partial trace

Let $C = A \otimes B = (A_{ij}B) \in M_m \otimes M_n$. $\qquad \sum q_i \rho_i \otimes \sigma_i$

$$\rho = \sum_{i=1}^{k} p_i |\psi_i\rangle\langle\psi_i| = \sum \tilde{p}_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum \lambda_i |\lambda_i\rangle\langle\lambda_i|$$

(1) One can take the partial trace of the first system to get the matrix B in the second system by simply summing the diagonal blocks of C resulting in $A_{11}B + \cdots + A_{mm}B = (\operatorname{tr} A)B = B$.

(2) One can take the partial trace of the second system to get the matrix A in the first system by simply taking the trace of all the blocks of C resulting in $(A_{ij}\operatorname{tr}(B)) = (A_{ij}) = A$.

For a general state $\rho = (T_{rs})_{1 \le r,s \le m}$ with $T_{rs} \in M_n$ for all r, s, the first partial trace and second partial traces are

$$\operatorname{tr}_1(\rho) = T_{11} + \cdots + T_{mm} \in M_n \quad \text{and} \quad \operatorname{tr}_2(\rho) = (\operatorname{tr} T_{ij}) \in M_m.$$

Let $A \in \mathcal{H}_1 \otimes \mathcal{H}_2$. The partial trace of A over $\mathcal{H}_2$ is an operator acting on $\mathcal{H}_1$ defined by

$$A_1 = \operatorname{tr}_2 A = \sum_{k=1}^{n} (I_m \otimes \langle e_{2,k}|) A (I_m \otimes |e_{2,k}\rangle),$$

$U|\psi\rangle\langle\psi|U^\dagger$

where m, n are the dimension of $\mathcal{H}_1$ and $\mathcal{H}_2$.

$\Phi(\rho) = U_t \rho U_t^\dagger$

In matrix form, if $\rho = (P_{ij}) \in M_m(M_n)$, then $\operatorname{tr}_2(\rho) = (\operatorname{tr} P_{ij}) \in M_n$. One can define $\operatorname{tr}_1(\rho_{ij}) = \rho_{11} + \cdots + \rho_{mm}$, which corresponds to

$$A_2 = \operatorname{tr}_1 A = \sum_{k=1}^{m} (\langle e_{1,k}| \otimes I_n) A (|e_{1,k}\rangle \otimes I_n).$$

Purification

Theorem Let $\rho_1 = \sum_{j=1}^{r} p_j |x_j\rangle\langle x_j|$. If $|\psi\rangle = \sum_{j=1}^{r} \sqrt{p_j} |x_j\rangle \otimes |y_j\rangle$, for an orthonromal set $\{|y_1\rangle, \dots, |y_r\rangle\} \subseteq \mathbb{C}^r$, then

$m \times m$

$$\mathrm{tr}_2(|\psi\rangle\langle\psi|) = \rho_1.$$

4×4 $\quad$ $A \otimes B$ $\quad$ $n \times n$

Example Let $\rho = \frac{1}{4}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} = \frac{3}{4}|x_1\rangle\langle x_1| + \frac{1}{4}|x_2\rangle\langle x_2|$ with

$$|x_1\rangle = (1,1)^t/\sqrt{2}, |x_2\rangle = (1,-1)^t/\sqrt{2}.$$

Let $\{|y_1\rangle, |y_2\rangle\} = \{|e_1\rangle, |e_2\rangle\}$.

Then $|\psi\rangle = \frac{1}{2\sqrt{2}}\begin{pmatrix} \sqrt{3} \\ 0 \\ \sqrt{3} \\ 0 \end{pmatrix} + \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}$ and

$$|\psi\rangle\langle\psi| = \frac{1}{8}\begin{pmatrix} 3 & \sqrt{3} & 3 & -\sqrt{3} \\ \sqrt{3} & 1 & \sqrt{3} & -1 \\ 3 & \sqrt{3} & 3 & -\sqrt{3} \\ -\sqrt{3} & -1 & -\sqrt{3} & 1 \end{pmatrix}.$$

$\frac{1}{2}\left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix}\right)\frac{1}{\sqrt{2}} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Dilation

Quantum operations on an open system

Quantum operations on a closed system with quantum state ρ has the form

$$\rho \mapsto U\rho U^{\dagger},$$

for some unitary U.

A quantum system ρ always interact with other quantum systems (from the environment or by the introduction of an auxiliary system for quantum computing).

We assume that σ is the quantum state for the environment or auxiliary system,

and the initial state of the open system is $\boxed{\sigma \otimes \rho}$.

Then a general quantum operation will be obtained by taking a suitable partial trace of $U(\sigma \otimes \rho)U^{\dagger}$.

$M_4 \to M_{\cancel{4}6}$

Theorem For every quantum operation on an open system $\Phi : M_n \to M_m$ there exist $r \in \mathbb{N}$ and $F_1, \dots, F_r \in M_{m,n}$ such that $\sum_{j=1}^r F_j^\dagger F_j = I_n$ and

$F_1^\dagger F_1 + \cdots + F_r^\dagger F_r = I_n$

and

$$\boxed{\Phi(A) = \sum_{j=1}^r F_j A F_j^\dagger} \qquad \text{for all } A \in M_n.$$

This is called the operator sum representation of the quantum operation. The matrices $F_1, \dots, F_r$ are called the Kraus operators of the operations.

Proof. Suppose $\Phi : M_n \to M_m$ is an quantum operation.

We may assume that $\Phi(\rho)$ is the partial trace of

$$U(\sigma \otimes \rho)U^\dagger \in M_{nk} \qquad \text{with } nk = mr.$$

Here U may depends on t. By purification, we may assume that $\sigma = E_{11}$ so that

$$U(\sigma \otimes \rho)U^\dagger = U \begin{pmatrix} \rho & 0 \\ 0 & 0 \end{pmatrix} U^\dagger = \begin{pmatrix} F_1 \\ \vdots \\ F_r \end{pmatrix} \rho (F_1^* | \cdots | F_r^*)$$

with diagonal blocks $F_1 \rho F_1^\dagger, \dots, F_r \rho F_r^\dagger$ so that

$$\boxed{\operatorname{tr}_1 (U(\sigma \otimes \rho)U^\dagger = \sum_{j=1}^r F_j \rho F_j^\dagger.}$$

Here $(F_1^\dagger, \dots, F_r^\dagger)$ are the first n rows of $U^\dagger$.

Thus, $\sum_{j=1}^r U_j^\dagger U_j = I_n$.

$F_j^\dagger F_j = I_n$

Example Let $U_1, \ldots, U_r \in \mathrm{U}(n)$ and $p_1, \ldots, p_r$ be positive numbers summing up to 1. Then $\Phi : M_n \to M_n$ defined by

$$\Phi(A) = \sum_{j=1}^{r} p_j U_j A U_j^\dagger \quad \text{for all } A \in M_n$$

is a quantum channel known as the **random unitary channel** or **mixed unitary channel**.

Quantum channels and Measurements

When a quantum state ρ is transmitted through a quantum channel, it will interact with the external environment. So, we may regard the transmission as a process of letting the quantum state going through a quantum operation of an open system, and assume the received state has the form

$$\hat{\rho} = \sum_{j=1}^{r} F_j \rho F_j^\dagger.$$

Here $F_1, \ldots, F_r$ are the Kraus operators caused by the influence of the environment on ρ. In this context, $F_1, \ldots, F_r$ are known a the **error operators**.

Positive Operator-Valued Measure (POVM)

- Eigenprojections of A.

  Quantum measurements can be viewed as quantum operations on open systems. As mentioned before a Hermitian matrix $A = \sum_{j=1}^{n} \lambda_j |\lambda_j\rangle\langle\lambda_j|$ is associated with an observable. If a state $\rho \in D_n$ goes through the measurement process corresponding to A, the state ρ will "collapse" to one of the pure states $|\lambda_j\rangle\langle\lambda_j|$ with a probability $\mathrm{tr}\,(A\rho)$.

- Projective measurement.

  In general, if $A = \sum_{j=1}^{s} \lambda_j P_j$, where P_j is the projection operator corresponding to the eigenvalue λ_j for the distinct eigenvalues $\lambda_1, \ldots, \lambda_s$ of A. In such a case, the **projective measurement** of ρ under the measurement associated with A is the quantum operation

$$\rho \mapsto \sum_j P_j \rho P_j,$$

  where $p_j = \mathrm{tr}\,(P_j \rho P_j) = \mathrm{tr}\,(\rho P_j)$ and the set $\{P_1, \ldots, P_r\}$ satisfies the completeness relation $\sum_j P_j P_j^\dagger = \sum_j P_j = I$.

- POVM. for any positive semidefinite matrices $Q_1, \dots, Q_r \in M_n$ such that $Q_1 + \cdots + Q_r = I_n$, there are $M_1, \dots, M_r \in M_n$ such that $M_j^\dagger M_j = Q_j$. The measurement operators are then associated with the quantum operation

$$\rho \mapsto \sum_{j=1}^{r} M_j \rho M_j^\dagger$$

so that ρ will change to the quantum state $\frac{1}{p_j} M_j \rho M_j^\dagger$ with a probability $p_j = \mathrm{tr}\,(M_j \rho M_j^\dagger) = \mathrm{tr}\,(\rho Q_j)$. The set $\{Q_1, \dots, Q_r\} = \{M_1^\dagger M_1, \dots, M_r^\dagger M_r\}$ is known as the **positive operator-valued measure (POVM)**.

Example Suppose Bob will be given a quantum state chosen from the linearly independent set of unit vectors $\{|\psi_1\rangle, \dots, |\psi_m\rangle\}$, which may not be orthonormal. He can construct the following POVM $\{Q_1, \dots, Q_{m+1}\}$ such that he will know for sure that $|\psi_j$ is sent to him if the measurement of the received state yields Q_j if $Q_j = |\phi_j\rangle\langle\phi_j|/m$, where $\langle\phi_j|\phi_j\rangle = 1$ and $\langle\phi_j|\psi_i\rangle = 0$ for all $i \neq j$ for $j = 1, \dots, m$ and $Q_{m+1} = I - \sum_{j=1}^{m} Q_j$. Evidently, a measurement of $|\psi_j\rangle\langle\psi_j|$ will yield Q_j or Q_{m+1}.

Fidelity

Definition 2.2 The fidelity of two density matrices ρ_1 and ρ_2 is defined as

$$F(\rho_1, \rho_2) = \operatorname{tr} \sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}}.$$

Note that $\sqrt{\rho_1}\rho_2\sqrt{\rho_1}$ is positive semidefinite so that $\sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}}$ is well defined and $F(\rho_1, \rho_2) = \operatorname{tr} \sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}} \geq 0$.

Example $\rho_1 = \operatorname{diag}(1/3, 2/3)$, $\rho_2 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$. Then

Remarks

1. If $A = \sum_j \lambda_j P_j$ with $\lambda_j \geq 0$, then $A^{1/2} = \sum_j \sqrt{\lambda_j} P_j$.

2. Let $R = \sqrt{\rho_1}\sqrt{\rho_2}$ with singular values $r_1, \ldots, r_n$. Then $RR^\dagger = \sqrt{\rho_1}\rho_2\sqrt{\rho_1}$ has eigenvalues $r_1^2, \ldots, r_n^2$ and

$$F(\rho_1, \rho_2) = \operatorname{tr}(\sqrt{RR^*}) = r_1 + \cdots + r_n.$$

3. Note also that $R^\dagger R$ also has the same eigenvalues $r_1^2 \geq \cdots \geq r_n^2$. So,

$$F(\rho_2, \rho_1) = \operatorname{tr}(R^* R) = \operatorname{tr} \sqrt{\sqrt{\rho_2}\rho_1\sqrt{\rho_2}} = r_1 + \cdots + r_n = F(\rho_1, \rho_2).$$

4. For any unitary U, $F(U\rho_1 U^\dagger, U\rho_2 U^\dagger) = F(\rho_1, \rho_2)$. (Exercise 2.10).

5. Suppose ρ_1, ρ_2 have eigenvalues $a_1 \geq \cdots \geq a_n$ and $b_1 \geq \cdots \geq b_n$. Then

$$F(\rho_1, \rho_2) = \max\{|\operatorname{tr}(\rho_1^{1/2}\rho_2^{1/2}U)| : U \text{ unitary}\} \leq \sum_{j=1}^n \sqrt{a_j b_j} \leq 1.$$

6. For any two density matrices ρ_1 and ρ_2, we have

$$0 \leq F(\rho_1, \rho_2) \leq 1.$$

The first equality holds if and only if $\rho_1\rho_2 = 0$; the second equality holds if and only if $\rho_1 = \rho_2$.

Open problems

1. Let $A \in D_m, B \in D_n$. Determine $\mathcal{S}(A, B) = \{C \in D_{mn} : \operatorname{tr}_1(C) = B, \operatorname{tr}_2(C) = A\}$.

2. Determine $C \in \mathcal{S}(A, B)$ with maximum rank and minimum rank.

3. Determine $C \in \mathcal{S}(A, B)$ with maximum $S(C) = \operatorname{tr}(-C \ln C)$, von Neumann entropy.

4. More generally, one may consider tripartite system with states in $D_{n_1 n_2 n_3}$ and determine $\mathcal{S}(T_1, T_2) = \{C \in D_{n_1 n_2 n_3} : \operatorname{tr}_1(C) = T_1, \operatorname{tr}_2(C) = T_2\}$, where $T_1 \in D_{n_2 n_3}$ and $T_2 \in D_{n_1 n_3}$ are two given states.