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Tutorial 12 (Schmidt decomposition and purifications[1])

(a) Prove the following theorem:

Theorem (**Schmidt decomposition**) Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_{\mathsf{A}}\rangle_{i=1,\dots,k}$ for system A, and orthonormal states $|i_{\mathsf{B}}\rangle_{i=1,\dots,k}$ for system B such that

$$|\psi\rangle = \sum_{i=1}^{k} \lambda_i \, |i_{\mathsf{A}}\rangle \, |i_{\mathsf{B}}\rangle \, ,$$

where λ_i are non-negative real numbers satisfying $\sum_{i=1}^{k} \lambda_i^2 = 1$ known as *Schmidt coefficients*.

(b) Show that, as consequence of the Schmidt decomposition, the deduced density matrices for subsystems A and B have the same eigenvalues if the composite system is in a pure state $|\psi\rangle$.

(c) Given a density operator ρ^{A} on a quantum system A, construct a pure state $|\psi\rangle$ on an extended quantum system AR such that $\rho^{\mathsf{A}} = \mathrm{tr}_{\mathsf{R}}[|\psi\rangle \langle\psi|]$. This procedure is known as *purification*.

Exercise 12.1 (Schmidt decomposition and entanglement entropy)
As in tutorial 12, let $|\psi\rangle$ be a pure state of a composite system, AB. The Schmidt decomposition of this state is denoted by $|\psi\rangle = \sum_{i=1}^{k} \sigma_i \, |i_{\mathsf{A}}\rangle \, |i_{\mathsf{B}}\rangle$.

(a) Verify that

$$\langle\psi|\psi\rangle = \sum_{i=1}^{k} \sigma_i^2.$$

In general, the *von Neumann entropy* of a density matrix ρ is defined as

$$\mathcal{S}(\rho) = -\,\mathrm{tr}[\rho \log(\rho)],$$

with the logarithm interpreted as matrix function, and the convention $0 \log(0) = \lim_{x\to 0} x \log(x) = 0$.

In tutorial 12 we found the reduced density matrices of the subsystems, defined as $\rho_1 = \mathrm{tr}_2[|\psi\rangle \langle\psi|]$ and $\rho_2 = \mathrm{tr}_1[|\psi\rangle \langle\psi|]$. We observed that ρ_1 and ρ_2 have the same eigenvalues $(\sigma_i^2)_{i=1,\dots,k}$. The *entanglement entropy* between the two subsystems is then given by

$$\mathcal{S}_{\mathsf{ent}} = \mathcal{S}(\rho_1) = \mathcal{S}(\rho_2) = -\sum_{i=1}^{k} \sigma_i^2 \log\bigl(\sigma_i^2\bigr).$$

(You should convince yourself that $\mathcal{S}(\rho_1)$ and $\mathcal{S}(\rho_2)$ are indeed equal to the sum on the right.) Intuitively, the entanglement entropy measures how strongly the subsystems are intertwined.

(b) Which sets of singular values $(\sigma_i)_{i=1,\dots,k}$ minimize and maximize the entanglement entropy, respectively, under the normalization condition $\sum_{i=1}^{k} \sigma_i^2 = 1$? ($k$ should be regarded as fixed.)
Hints: The smallest possible entanglement entropy is zero. Regarding maximization, you can take the normalization condition via a Lagrange multiplier into account.

(c) Show that $\mathcal{S}_{\mathsf{ent}} = 0$ (completely unentangled case) implies that $|\psi\rangle$ can be written as tensor product of a state from subsystem A and one from subsystem B.

[1] M. A. Nielsen, I. L. Chuang: *Quantum Computation and Quantum Information*. Cambridge University Press (2010), Section 2.5

Exercise 12.2 (Python/NumPy implementation of the partial trace)

(a) Implement the partial trace operation for arbitrary dimensions using Python/NumPy. Specifically, you should write a function with signature `partial_trace(rho, dimA, dimB)`, where `rho` is the density matrix of the composite quantum system, and `dimA`, `dimB` specify the dimensions of subsystems A and B, respectively. (Thus `rho` is a `dimA`$\cdot$`dimB` $\times$ `dimA`$\cdot$`dimB` matrix.) The function should return a tuple $(\rho^{\mathsf{A}}, \rho^{\mathsf{B}})$ containing the reduced density matrices $\rho^{\mathsf{A}} = \mathrm{tr}_{\mathsf{B}}[\mathtt{rho}]$ and $\rho^{\mathsf{B}} = \mathrm{tr}_{\mathsf{A}}[\mathtt{rho}]$.

Hint: First reshape `rho` into a `dimA` $\times$ `dimB` $\times$ `dimA` $\times$ `dimB` tensor using `numpy.reshape`. Then apply `numpy.trace` to trace out certain dimensions.

(b) Apply your function to $\rho = |\psi\rangle\langle\psi|$ with the Bell state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. The reduced density matrices should both be equal to $\frac{I}{2}$.

Hint: Represent $|\psi\rangle$ as vector (NumPy array) of length 4. `numpy.outer(psi, psi.conj())` computes the outer product $|\psi\rangle\langle\psi|$.

(c) Test your implementation by constructing a random density matrix ρ on the composite system and a random observable M on subsystem A, and then numerically verifying that $\mathrm{tr}[M\rho^{\mathsf{A}}] = \mathrm{tr}[(M \otimes I)\rho]$ (up to numerical rounding errors).

You can use the following functions to obtain ρ and M:

```
import numpy as np


def construct_random_density_matrix(d):
    """
    Construct a complex random density matrix of dimension d x d.
    """
    # ensure that rho is positive semidefinite
    A = (np.random.randn(d, d) + 1j*np.random.randn(d, d))/np.sqrt(2)
    rho = A @ A.conj().T
    # normalization
    rho /= np.trace(rho)
    return rho


def construct_random_operator(d):
    """
    Construct a complex random Hermitian matrix of dimension d x d.
    """
    # ensure that M is Hermitian
    A = (np.random.randn(d, d) + 1j*np.random.randn(d, d))/np.sqrt(2)
    M = 0.5*(A + A.conj().T)
    return M
```

Hint: In Python $\geq$ 3.5, the `@` operator performs the matrix product.