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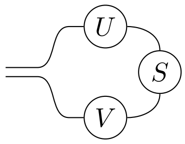
Exercise 8.1 (Schmidt decomposition and entanglement entropy)
Let $\psi \in \mathbb{C}^{m \cdot n}$ be a complex vector. We may interpret ψ as $m \times n$ matrix and compute its SVD, for which we use the convention $\psi = USV^T$ here, with isometries $U \in \mathbb{C}^{m \times k}$, $V \in \mathbb{C}^{n \times k}$ (such that $U^\dagger U = I$ and $V^\dagger V = I$), $k = \min(m, n)$ and $S = \mathrm{diag}(\sigma_1, \dots, \sigma_k)$. (The V matrix appears without complex conjugation in the SVD.) As graphical diagram:

ψ =


(a) Show that

$$\|\psi\|^2 = \sum_{j=1}^{k} \sigma_j^2.$$

Hint: Revisit the definition and properties of the Frobenius norm, or use the diagrammatic representation.

(b) The partial trace has been introduced in Exercise 5.1. Here the two subsystems have dimension m and n, respectively. Verify that

$$\mathrm{tr}_2[\psi \circ \psi^*] = US^2U^\dagger \quad \text{and}$$
$$\mathrm{tr}_1[\psi \circ \psi^*] = VS^2V^\dagger.$$

In part (b) we have thus found the spectral decompositions of the "reduced density matrices" defined as $\rho_1 = \mathrm{tr}_2[\psi \circ \psi^*]$ and $\rho_2 = \mathrm{tr}_1[\psi \circ \psi^*]$ (potentially omitting zero eigenvalues). One observes that ρ_1 and ρ_2 have the same (non-zero) eigenvalues $(\sigma_j^2)_{j=1,\dots,k}$. In the following, we assume that $\|\psi\| = 1$, such that $\sum_{j=1}^k \sigma_j^2 = 1$ according to (a).

In general, a density matrix ρ is a Hermitian, positive semidefinite matrix with normalization $\mathrm{tr}[\rho] = 1$. The *von Neumann entropy* of 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 the present setting, the *entanglement entropy* between the two subsystems is defined as

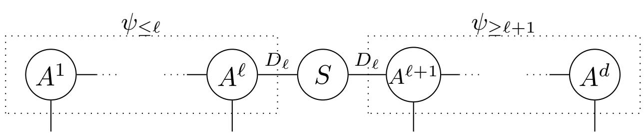
$$\mathcal{S}_{\mathrm{ent}} = \mathcal{S}(\rho_1) = \mathcal{S}(\rho_2) = -\sum_{j=1}^{k} \sigma_j^2 \log\big(\sigma_j^2\big).$$

(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.

(c) Which singular values $(\sigma_j)_{j=1,\dots,k}$ minimize and maximize the entanglement entropy, respectively, under the normalization condition $\sum_{j=1}^k \sigma_j^2 = 1$? ($k$ should be regarded as given and fixed.)

Hint: The smallest possible entanglement entropy is zero. Regarding maximization, first consider the case $k = 2$.

(d) Finally, we consider the case that ψ is represented in bond-canonical MPS form, for some $\ell \in \{1, \dots, d-1\}$:

ψ =


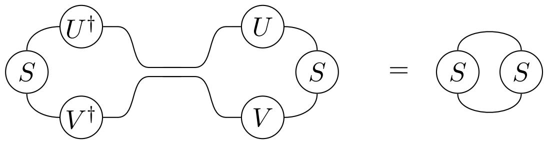
Here the tensors A^j for $j = 1, \dots \ell$ are left-orthonormal, the tensors A^j for $j = \ell + 1, \dots, d$ are right-orthonormal, and S is the diagonal matrix of "bond" singular values. In the above setting, the first ℓ open (downward-pointing) legs form subsystem 1, and correspondingly the remaining legs subsystem 2. When denoting the dimensions of the open legs by $n_1, \dots, n_d$, then $m = n_1 \cdots n_\ell$ and $n = n_{\ell+1} \cdots n_d$. Show that the tensor $\psi_{\leq \ell}$ (interpreted as $m \times D_\ell$ matrix) and the transpose of $\psi_{\geq \ell+1}$ (interpreted as $D_\ell \times n$ matrix) are both isometries.

Remark: The bond-canonical MPS representation can thus be interpreted as SVD of ψ, where $\psi_{\leq \ell}$ plays the role of the above U and $\psi_{\geq \ell+1}^T$ the role of the above V. In particular, the "bond" singular values determine the entanglement entropy.

Solution

(a) We can visualize the operation as an inner product, noting that U and V are unitary matrices and that S is a real, diagonal matrix.

$$\|\psi\|^2 = \langle \psi, \psi \rangle =$$

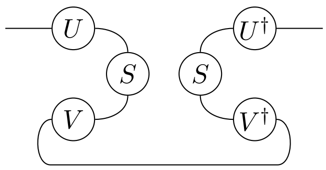


This simplifies to $\|\psi\|^2 = \sum_{j=1}^{k} \sigma_j^2$.
Alternatively, we can use the unitary invariance of the Frobenius norm:

$$\|\psi\|^2 = \|USV^T\|_F^2 = \|S\|_F^2 = \sum_{j=1}^{k} \sigma_j^2.$$

(b) We draw the graphical representation of the outer product and trace out the second qubit:

$$\mathrm{tr}_2[\psi \circ \psi^*] =$$

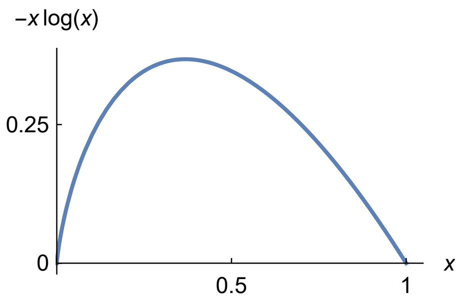


Since $V^\dagger V = I$, the V matrices drop out, which leads to

$$\mathrm{tr}_2[\psi \circ \psi^*] = US^2U^\dagger.$$

The relation $\mathrm{tr}_1[\psi \circ \psi^*] = VS^2V^\dagger$ follows analogously.

(c) We know that singular values are (in general) real and non-negative. Moreover, due to the normalization condition, $\sigma_j^2 \in [0, 1]$ for all $j = 1, \ldots, k$. The following figure visualizes $-x \log(x)$, which is non-negative for any $x \in [0, 1]$, and equal to 0 precisely if $x = 0$ or $x = 1$.



By identifying x with σ_j^2, one concludes that the entanglement entropy is non-negative. $\mathcal{S}_{\mathrm{ent}} = 0$ is reached by setting one of the singular values to 1 and the others to 0 (which satisfies the normalization condition).

Regarding maximization of the entanglement entropy, we take the normalization constraint by a Lagrange multiplier $\lambda \in \mathbb{R}$ into account, and abbreviate $\sigma_j^2 = x_j$ for convenience:

$$\mathcal{L}(x_1, \ldots, x_k, \lambda) = -\sum_{j=1}^{k} x_j \log(x_j) - \lambda \left(\sum_{j=1}^{k} x_j - 1 \right).$$

Finding an extremum of $\mathcal{L}$ by differentiation w.r.t. x_j, and using that $\log'(x) = \frac{1}{x}$ for $x > 0$, gives

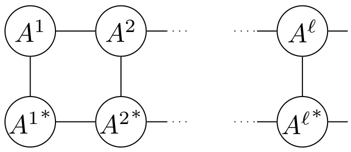
$$0 \stackrel{!}{=} \frac{\partial \mathcal{L}}{\partial x_j} = -\log(x_j) - 1 - \lambda \quad \rightsquigarrow \quad x_j = e^{-1-\lambda}.$$

In particular, all x_j take the same value; combined with the normalization condition, one arrives at $x_j = \frac{1}{k}$ for all $j = 1, \ldots, k$. This assignment indeed maximizes $\mathcal{L}$ since $-x \log(x)$ is concave. The corresponding singular values are $\sigma_j = \frac{1}{\sqrt{k}}$ for $j = 1, \ldots, k$, and

$$\max_{\sigma_1, \ldots, \sigma_k} \mathcal{S}_{\mathrm{ent}} = -\log(1/k) = \log(k).$$

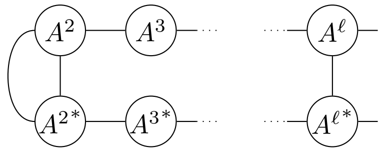
(d) In order to show that $\psi_{\leq \ell}$ is an isometry, we contract it with its conjugate transpose:

$${\psi_{\leq \ell}}^{\dagger}\, \psi_{\leq \ell} \;=$$

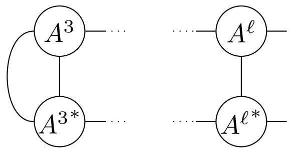


Now we repeatedly exploit the left-orthonormality of the A^j tensors to arrive at:

$$\psi_{\leq \ell}^{\dagger}\, \psi_{\leq \ell} \;=$$



$$=$$



$$= \;\dots\; =$$

This graphical diagram corresponds to the equation

$$\psi_{\leq \ell}^{\dagger} \psi_{\leq \ell} = I_{D_\ell},$$

which is precisely the definition of an isometry.

The derivation for the transpose of $\psi_{\geq \ell+1}$ proceeds analogously.

Remark: The left-orthonormality of the A^j tensors can also be interpreted as follows: the vectorized identity matrix is a left-eigenvector of the transfer operator corresponding to A^j, with eigenvalue 1 (cf. Tutorial 10).