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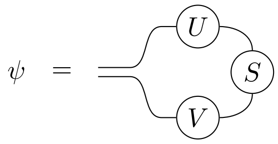
Exercise 8.1 (Schmidt decomposition and entanglement entropy)
Let $\psi \in \mathbb{C}^{m \cdot n}$ be a complex vector. We may interpret ψ as $m \times n$ matrix and compute its SVD, for which we use the convention $\psi = USV^T$ here, with isometries $U \in \mathbb{C}^{m \times k}$, $V \in \mathbb{C}^{n \times k}$ (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:



(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).

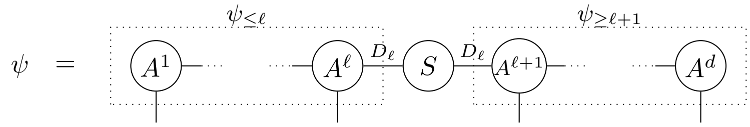
In general, a density matrix ρ is a Hermitian, positive semidefinite matrix with normalization $\mathrm{tr}[\rho] = 1$. The *von Neumann entropy* of ρ is defined as
$$\mathcal{S}(\rho) = -\,\mathrm{tr}[\rho \log(\rho)],$$
with the logarithm interpreted as matrix function, and the convention $0 \log(0) = \lim_{x \to 0} x \log(x) = 0$.

In the present setting, the *entanglement entropy* between the two subsystems is defined as
$$\mathcal{S}_{\mathrm{ent}} = \mathcal{S}(\rho_1) = \mathcal{S}(\rho_2) = -\sum_{j=1}^{k} \sigma_j^2 \log\bigl(\sigma_j^2\bigr).$$

(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.

(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 $\ell \in \{1, \dots, d-1\}$:



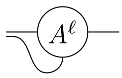
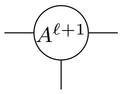
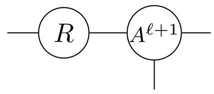
Here the tensors A^j for $j = 1, \dots \ell$ are left-orthonormal, the tensors A^j for $j = \ell+1, \dots, d$ are right-orthonormal, and S is the diagonal matrix of "bond" singular values. In the above setting, the first ℓ open (downward-pointing) legs form subsystem 1, and correspondingly the remaining 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 $\psi_{\le \ell}$ (interpreted as $m \times D_\ell$ matrix) and the transpose of $\psi_{\ge \ell+1}$ (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 $\psi_{\le \ell}$ plays the role of the above U and $\psi_{\ge \ell+1}^T$ the role of the above V. In particular, the "bond" singular values determine the entanglement entropy.

Exercise 8.2 (Canonical MPS forms)
The goal of this exercise is to covert a MPS into several canonical forms. We first revisit left-orthonormalization: compared to the lecture, one can bring the last tensor into left-orthonormal form, too, by introducing an additional trailing (dummy) tensor $A^{d+1} \in \mathbb{R}^{1\times1\times1}$, which absorbs the final R matrix. This R matrix is in $\mathbb{R}^{1\times1}$, since $D_d = 1$ and the diagonal entries of R are real-valued in general. The single entry of A^{d+1} is the overall (Frobenius) norm of the input MPS, and returned by the following algorithm. Note that the overall norm of the updated MPS is equal to 1 since all tensors are left-orthonormal.

Left-orthonormalization of a matrix product state

Input: list of MPS tensors $A^\ell \in \mathbb{C}^{n_\ell\times D_{\ell-1}\times D_\ell}$, $\ell = 1,\dots,d$
(with singleton bond dimensions $D_0 = D_d = 1$)

1. Define an additional (temporary) tensor $A^{d+1} \in \mathbb{R}^{1\times1\times1}$ with single entry 1
2. `for` $\ell = 1,\dots,d$:
   Reshape A^ℓ into a $(n_\ell D_{\ell-1}) \times D_\ell$ matrix, and
   compute the ("economy-size") QR-decomposition  $= QR$
   Update $D^\ell \leftarrow$ second dimension of Q, and $A^\ell \leftarrow \text{reshape}(Q,(n_\ell, D_{\ell-1}, D_\ell))$
   Absorb R into the next tensor:  $\leftarrow$ 
3. In case the single entry of A^{d+1} is negative, flip the signs of A^d and A^{d+1}
4. `return` list of updated tensors $(A^\ell)_{\ell=1,\dots,d}$, and the single entry of A^{d+1} (Frobenius norm of input MPS)

The Moodle page contains a Jupyter notebook template for this exercise, with placeholders for the following parts:

(a) Implement the above algorithm for left-orthonormalization in the function
`mps_orthonormalize_left(Alist)`

Hint: For the QR-decompositions you can use `np.linalg.qr(..., mode='reduced')`. It is not necessary to store a list of virtual bond dimension D_ℓ, since these can be obtained from the dimensions of the NumPy arrays A^ℓ.

(b) Implement an analogous algorithm for right-orthonormalization in the function
`mps_orthonormalize_right(Alist)`

Hint: Conceptually, this is the same algorithm as left-orthonormalization after left-right mirroring.

(c) Implement the function `mps_orthonormalize_center(Alist, j)` for converting a MPS to *site-canonical form* with center at site `j`, such that all tensors to the left are left-orthonormal, and all tensors to the right are right-orthonormal. (The center tensor A^j needs not be of any normal form.)

(d) Implement the function `mps_orthonormalize_bond(Alist, j)` to convert a MPS into bond-canonical form as discussed in Exercise 8.1(d) above. The function should return the list of "bond" singular values.

Hint: You can first convert to site-canonical form with center at j, and then update the tensors A^j and A^{j+1}.

(e) Finally, run the notebook using your implementations, ensuring that all consistency checks pass.