Responsible TA: Brandon Barton, bbarton@phys.ethz.ch
Exercise class in HCI J7.

Exercise 1. *MPS and MPO representations*

The goal of this exercise is to find Matrix Product State (MPS) and Matrix Product Operator (MPO) expressions of particular states and the Heisenberg Hamiltonian (analytically).

1. Find a set of MPS tensors encoding the state

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|01010...\rangle + |10101...\rangle), \tag{1}$$

   for N spins. Distinguish between even and odd number of spins.

   Hint. Modify the MPS representation of the GHZ state discussed in the lecture.

2. Find the MPS representation of the state

$$|\Psi_2\rangle = \frac{1}{(\sqrt{2})^N}(|0\rangle + |1\rangle)^{\otimes N}, \tag{2}$$

   with N an arbitrary number of spins.

3. It has been discussed in the lecture that an MPS can be written in Vidal's canonical form:

$$|\Psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \Lambda^{[0]}\Gamma^{[1]\sigma_1}\Lambda^{[1]}\Gamma^{[2]\sigma_2}\Lambda^{[2]}\ldots\Lambda^{[N-1]}\Gamma^{[N]\sigma_N}\Lambda^{[N]}, \tag{3}$$

   where $\Lambda^{[i]}$ are diagonal matrices. For a system with open boundary conditions, $\Lambda^{[0]}$ and $\Lambda^{[N]}$ are scalars and determine the normalization. We can normalize the wavefunction by setting them to 1. Interestingly, the diagonal entries of the matrix $\Lambda^{[i]}$ correspond to the Schmidt values of a bipartion of the system between sites i and $i+1$.

4. Find the canonical form of the MPS representation of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$.

5. (Optional) Operators can be represented as Matrix Product Operators (MPO). Find a set of MPO tensors representing the Heisenberg Hamiltonian

$$H = -J\sum_i \hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1}. \tag{4}$$

Exercise 2. *Canonization and overlaps*

The goal of this exercise is to implement various procedures for computations with MPS and MPO. Many calculations are simpler when working in the Vidal's canonical form (4), so we will first implement a canonization procedure.

Hint. you might find the following numpy functions useful: *np.dot, np.tensordot, np.reshape, np.transpose, np.conj, np.linalg.svd*.

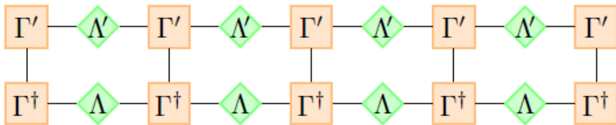
1. Implement a procedure that, given a MPS representation $M = [M^{[1]\sigma_1}, ..., M^{[N]\sigma_N}]$, computes the left-normalized representation $[A^{[1]}, ..., A^{[n]}]$. Do the same for the right-normalized representation $[B^{[1]}, ..., B^{[n]}]$.

2. Given a general (non-canonical) MPS representation $M = [M^{[1]\sigma_1}, ..., M^{[N]\sigma_N}]$ of a state $|\Psi\rangle$, write a function that constructs the Vidal canonical form and returns the matrices $\Gamma = [\Gamma^{[1]\sigma_1}, ..., \Gamma^{[N]\sigma_N}]$ and $\Lambda = [\Lambda^{[1]}, ..., \Lambda^{[N-1]}]$. Use the implemented function to determine the Vidal canonical form of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ introduced in exercise 1 and compare to your result of exercise 1.4.

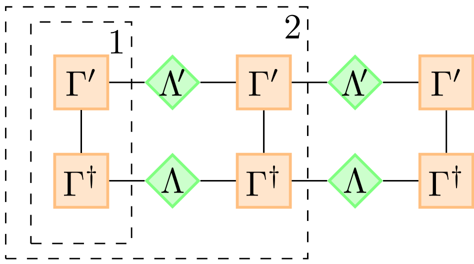
   Hint. First right-normalize the state and then run a left-normalization procedure where you factor out the singular values Λ, as discussed in the lecture.

In the following, we assume that the MPS are in Vidal's canonical form. We start by evaluating the overlap between two states:

$\langle\Psi|\Psi'\rangle =$



We efficiently evaluate the overlap by iteratively contracting the matrices, starting from the left and contracting one more site in each step. The first two steps of the iteration process are depicted in the following diagram:



Step 2 is repeated until the last site is reached. Equivalently, one can start at the rightmost site and contract from the right to the left.

3. What would be the complexity (i.e. the number of terms) of the contraction operation, if we would first contract all matrix indices (horizontal legs in the diagram) and then all physical indices (vertical legs in the diagram)?

4. Given MPS representations of two states $|\Psi\rangle$ and $|\Psi'\rangle$ in Vidal's canonical form $[\Gamma^{[1]\sigma_1}, ..., \Gamma^{[N]\sigma_N}]$, $[\Lambda^{[1]}, ..., \Lambda^{[N-1]}]$ and $[\Gamma'^{[1]\sigma_1}, ..., \Gamma'^{[N]\sigma_N}]$ and $[\Lambda'^{[1]}, ..., \Lambda'^{[N-1]}]$ write a function that evaluates their overlap $\langle\Psi|\Psi'\rangle$ as described above. Calculate the overlap between $|\Psi_1\rangle$ and $|\Psi_2\rangle$ for $N = 30$ spins. Verify the correct implementation of your function by calculating the normalization of an arbitrary MPS state in canonical form (should be equal to 1).