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Exercise class in HCI J7.

Exercise 1. *MPS of spin systems*

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

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

2. Using the code from last week, implement the transverse-field Ising model without periodic boundary conditions (i.e., open boundary conditions)

$$H = -\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h \sum_i \hat{\sigma}_i^x$$

in MPO form. The MPO form of the transverse-field Ising model (without periodic boundary conditions) can be found in the lecture notes.

Exercise 2. *Expectation values of MPOs*

We want to evaluate expectation values of Matrix Product Operators, $\langle\Psi|O|\Psi\rangle$. They can be evaluated using the same procedure as for overlaps of MPS (which we have seen last week): starting from either the left or the right and iteratively contracting the matrices. We will work in Vidal's canonical form as we did last week.

1. How would you graphically represent the expectation value $\langle\Psi|O|\Psi\rangle$ using the diagrammatic tensor network notation?
2. Given the transverse-field Ising model

$$H = \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h \sum_i \hat{\sigma}_i^x \tag{1}$$

calculate the variational energy $\langle\Psi|H|\Psi\rangle / \langle\Psi \mid \Psi\rangle$ for the states

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|01010\ldots\rangle + |10101\ldots\rangle) \text{ and } |\Psi_2\rangle = \frac{1}{\sqrt{2}^N}(|0\rangle + |1\rangle)^{\otimes N} \tag{2}$$

for $N = 30$ spins at the values $h = 0, h = 1$ and $h = 2$ and explain the outcome. The result can be easily verified analytically. Compare the obtained variational energies with the variational energies obtained using a randomly generated MPS with bond dimension $\chi = 2$. We will make use of the variational energy in the next question!

Hint: use the MPO form of the transverse-field Ising model discussed in the lecture.

Exercise 3. ***DMRG implementation***

The goal of this exercise is to implement the single-site DMRG algorithm in order to obtain the ground state of the transverse field Ising model with open boundary conditions. To recall, DMRG minimizes the energy expectation value

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi \mid \psi\rangle}$$

with respect to the MPS matrices $\{M_1^{\sigma_1}, M_2^{\sigma_2}, \ldots\}$. The single-site DMRG is a variational method that optimizes the ground state energy locally, changing only one MPS tensor at a time.

We start by creating a random MPS and right-normalizing it. We also need the MPO of the transverse field Ising Hamiltonian. These are two ingredients needed as an input to the actual DMRG. The DMRG algorithm on a chain of size N consists of left and right sweeps during which the energy as well as the MPS get evaluated locally, as described by the pseudocode in the following

Input: MPS, MPO, tolerance
Consecutively compute all right environments R
while energy is converged = False **do**
Initialize current left environment L = np . ones((1, 1, 1))
for i **in** range(N − 1) **do**

1. Initialize local operator $\hat{\mathcal{H}}$ acting on a site i with the correct dimensions for M^i using MPO, left and right environments $L[i]$ and $R[L-1$ - i] (use `scipy.sparse.linalg.LinearOperator`).
2. Obtain local energy and optimal M^i diagonalizing $\hat{\mathcal{H}}M^i = \lambda M^i$ (`scipy.sparse.linalg.eigsh`).
3. Left-normalize M^i, namely $M^i \to A^i$. Note also that M^{i+1} will also be affected and lose its normalization, but it will just be used as an initial guess for the next optimization.

Repeat the same procedure now for the right sweep.
Store energies from both sweeps.
end for
The algorithm stops when the energy is converged or the energy variance drops below a certain threshold.
end while

Remarks

1. Routines to create a random MPS, right-normalize and left-normalize it were already found in last week's exercise - these will be given to you. The MPO representation of the transverse field Ising model can be reused from Exercise 2.

2. You will need to write the functions that compute left environment and right environment. To better understand the contraction indices, please refer to this week's manuscript.

3. Finally, recall that the optimization problem solved in DMRG is

$$\sum_{\sigma_l a_{l-1} a_l} \Big(\underbrace{\sum_{b_l b_{l-1}} L_{a_{l-1} b_{l-1} a'_{l-1}} W^{\sigma'_l \sigma_l}_{b_{l-1} b_l} R_{a_l b_l a'_l}}_{\hat{\mathcal{H}}} \Big) M^{\sigma_l}_{a_{l-1} a_l} = \lambda M^{\sigma'_l}_{a'_{l-1} a'_l}$$

This expression is valid only if right and left environments were obtained for correctly canonized MPS. The under-braced expression is the local "Hamiltonian" acting on the MPS matrix at site l. The construction of this Hamiltonian itself is very inefficient, so you should define a function that produces the action of the Hamiltonian on $M^{[i]}$, given $M^{[i]}$ and environments $L^{[i]}, R^{[i]}$. This function is passed to `scipy.sparse.linalg.LinearOperator` to create a Linear Operator object. You can then solve the eigenvalue problem using the Lanczos algorithm.