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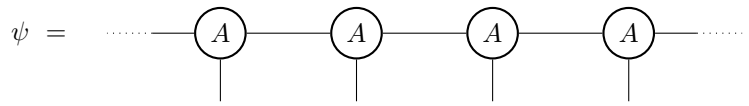
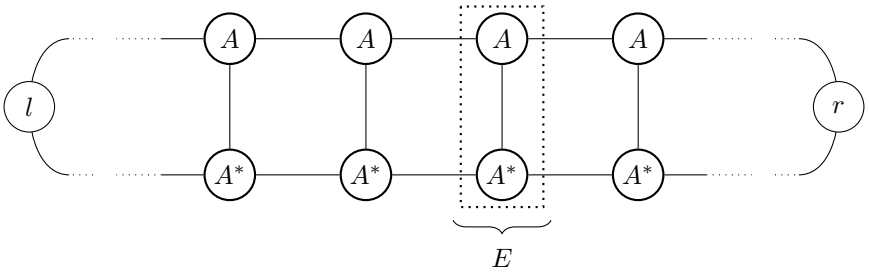
Tutorial 10 (Infinite MPS[1])

When investigating large systems, it is often easier to work directly in the "thermodynamic limit" $L \to \infty$ (with L the system size, like number of lattice sites). Typical quantum Hamiltonians are translation invariant (i.e., their mathematical form remains invariant when shifting lattice site labels), which motivates a likewise translation invariant MPS Ansatz for a quantum state ψ, i.e., using the same tensor at each site. Taken together, this leads to the following iMPS form:



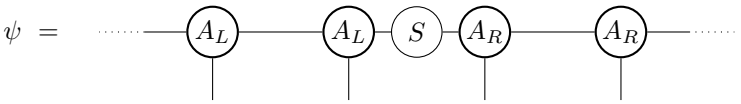
(a) While the MPS is uniquely defined by the tensor A, show that the converse is not true. This is denoted a gauge degree of freedom.

To compute expectation values of observables using an iMPS (see below) and ensure it is properly normalized, one imagines that a contraction for computing $\langle \psi, \psi \rangle$ starts "infinitely" at the right and then proceeds to the left (or other way around). Recall from Exercise 6.2 that a single step involves multiplication with the *transfer matrix* E. Identifying the repeated application of E as power iteration, this procedure will single out the eigenvector (denoted r) of E corresponding to its largest (in absolute value) eigenvalue. Equivalently, one can start "infinitely" at the left, which will tend to the left-eigenvector l of E corresponding to its largest eigenvalue.



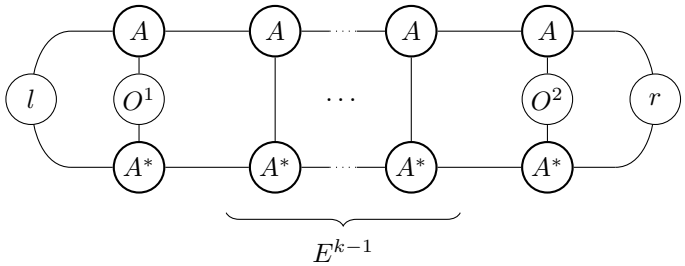
(b) Represent the eigenvalue equations as tensor diagrams. Which value must the largest eigenvalue of E have to ensure normalization of ψ? Explain how we finally arrive at $\langle \psi, \psi \rangle = \mathrm{tr}[lr]$.

(c) It turns out that l and r can be chosen as positive definite matrices. Use this property and the gauge freedom from (a) to bring the iMPS into the following bond-canonical form, where A_L is left-orthonormal and A_R right-orthonormal, and S a diagonal matrix of singular values:



(d) Let O_j be an observable acting on a single lattice site j. (Due to translation invariance it is irrelevant which one.) Express the expectation value $\langle \psi, O_j \psi \rangle$ in terms of the iMPS tensors, both for the uniform version (same tensor A at each site) and the bond-canonical form in (c).

(e) Much insight into a quantum system can be gained from correlation functions, i.e., observables of the form $O_j^1 O_{j+k}^2$ which are k sites apart. Use the spectral decomposition of the transfer operators E to simplify the following tensor network contraction for evaluating $\langle \psi, O_j^1 O_{j+k}^2 \psi \rangle$:

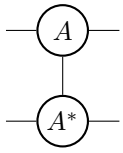


[1] Tutorial based on: L. Vanderstraeten, J. Haegeman, F. Verstraete: *Tangent-space methods for uniform matrix product states*, SciPost Phys. Lect. Notes 7 (2019) (arXiv:1810.07006)

Exercise 10.1 (Properties of the AKLT state)
We can use the methods from Tutorial 10 to analyze the AKLT state, denoted ψ here. First recall that its MPS tensors $A \in \mathbb{C}^{3\times 2\times 2}$ (which are both left- and right-orthonormal) are given by

$$A_{\hat{1},:,:} = \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{pmatrix}, \quad A_{\hat{0},:,:} = \begin{pmatrix} -\sqrt{\frac{1}{3}} & 0 \\ 0 & \sqrt{\frac{1}{3}} \end{pmatrix}, \quad A_{-\hat{1},:,:} = \begin{pmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{pmatrix}.$$

(a) Calculate the corresponding 4×4 transfer matrix

$E =$ 

$= \sum_{\sigma\in\{1,0,-1\}} A_{\hat{\sigma},:,:} \otimes A^*_{\hat{\sigma},:,:},$

and compute its spectral decomposition. Why can we infer from the orthonormalization of the MPS tensors that the largest eigenvalue of E must be 1?

(b) It turns out that the AKLT state has a "hidden order", which is indicated by fact that the "string correlation function" $\langle \psi, S^z_j \left(\prod_{j<\ell<j+k} \mathrm{e}^{i\pi S^z_\ell} \right) S^z_{j+k} \psi \rangle$ does not tend to 0 with increasing k. Draw the tensor diagram for evaluating this correlation function.

(c) (Voluntary) Evaluate the string correlation function symbolically for arbitrary integer $k \geq 2$.

Hint: You can use a symbolic algebra system like Wolfram Alpha (wolframalpha.com) or Mathematica to solve this task. Your final result should be independent of k.

Exercise 10.2 (MPO representation of a quantum Hamiltonian)
In the lecture we have discussed how a Hamiltonian with local terms on a one-dimensional lattice can be represented exactly as matrix product operator (MPO). Use the Jupyter notebook template from the Moodle page to complete the following tasks.

(a) Recall the transverse-field Ising Hamiltonian on a one-dimensional lattice with open boundary conditions:

$$H_{\text{ising}} = -J \sum_{j=1}^{L-1} Z_j Z_{j+1} - g \sum_{j=1}^{L} X_j,$$

where $J, g \in \mathbb{R}$ are parameters and L denotes the number of lattice sites. Implement the function `construct_ising_hamiltonian_mpo(J, g, L, pbc=False)` to generate the corresponding MPO tensors

$$A^1 = \begin{pmatrix} -gX & -JZ & I_2 \end{pmatrix}, \quad A^j = \begin{pmatrix} I_2 & 0 & 0 \\ Z & 0 & 0 \\ -gX & -JZ & I_2 \end{pmatrix} \ \forall j = 2, \ldots, L-1, \quad A^L = \begin{pmatrix} I_2 \\ Z \\ -gX \end{pmatrix},$$

where the zero entries stand for 2×2 zero matrices. The function should return $(A^j)_{j=1,\ldots,L}$ as a list. You can ignore the case `pbc=True` here, which is only relevant for the voluntary part (c).

To test your implementation, use the notebook template to convert the MPO to a full tensor (by contracting the virtual bonds), and ensure this agrees with the direct sparse matrix construction of the Hamiltonian provided in the notebook.

Hint: You can literally assemble the A^j tensors as "array of arrays" using NumPy, but then still have to transpose dimensions such that $A^j \in \mathbb{C}^{2\times 2\times D_{j-1}\times D_j}$.

(b) We now consider the so-called cluster state Hamiltonian on a one-dimensional lattice with L sites:

$$H_{\text{cluster}} = -J \sum_{j=2}^{L-1} Z_{j-1} X_j Z_{j+1}.$$

What are corresponding MPO tensors for representing this Hamiltonian? Assemble these by implementing the function `construct_cluster_hamiltonian_mpo(J, L)`.

Hint: The finite state automaton should consist of four states.

(c) (Voluntary) Assuming that the leftmost and rightmost virtual bonds with respective dimensions D_0 and D_L are allowed to be larger than 1 and are contracted, how can one modify the MPO tensor A^1 and A^L to represent the Ising Hamiltonian on a 1D lattice with *periodic* boundary conditions?

Extend your implementation of `construct_ising_hamiltonian_mpo(J, g, L, pbc=False)` accordingly to handle the case `pbc=True` as well.