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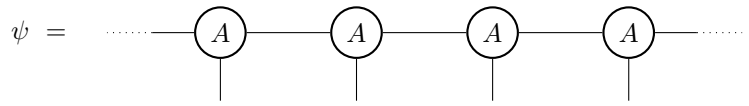
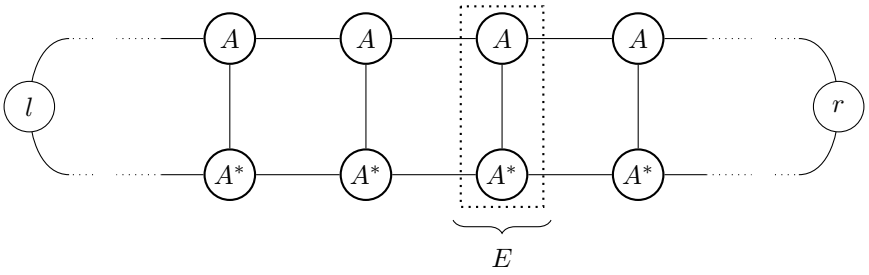
Tutorial 10 (Infinite MPS[1])
When investigating large systems, it is often easier to work directly in the "thermodynamic limit" $L \to \infty$ (with L the system size, like number of lattice sites). Typical quantum Hamiltonians are translation invariant (i.e., their mathematical form remains invariant 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:



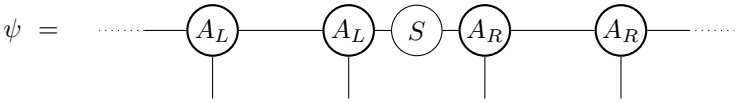
(a) While the MPS is uniquely defined by the tensor A, show that the converse is not true. This is denoted a gauge degree of freedom.

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.



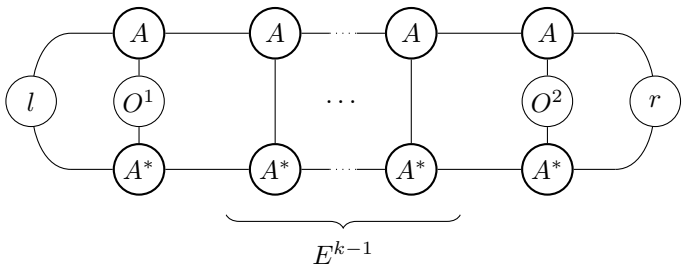
(b) Represent the eigenvalue equations as tensor diagrams. Which value must the largest eigenvalue of E have to ensure normalization of ψ? Explain how we finally arrive at $\langle \psi, \psi \rangle = \mathrm{tr}[lr]$.

(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).

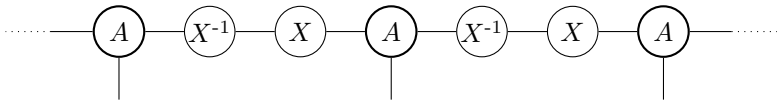
(e) Much insight into a quantum system can be gained from correlation functions, i.e., observables of the form $O_j^1 O_{j+k}^2$ which are k sites apart. Use the spectral decomposition of the transfer operators E to simplify the following tensor network contraction for evaluating $\langle \psi, O_j^1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



[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)

Solution

(a) We can insert any invertible matrix X and its inverse between bond connections:



From this form we see that the new uniform tensor A', defined by $A'_{s,:,:} = XA_{s,:,:}X^{-1}$ for all s, gives rise to the same overall quantum state.

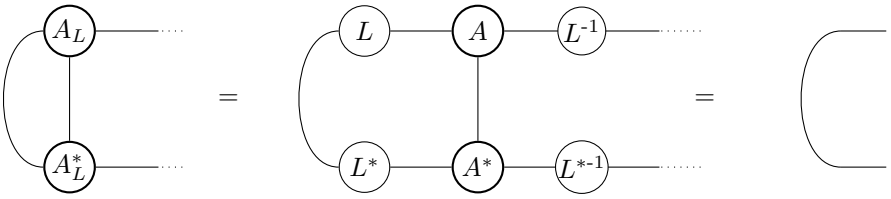
(b) In order for the power iteration to converge to a fixed point, the largest eigenvalue of E must be 1. Note that E and E^T have the same eigenvalues (which holds in general for any square matrix and can be seen from the characteristic polynomial), i.e., the "left" eigenvalues agree with the "right" eigenvalues.

The eigenvector relations (for eigenvalue 1) can be expressed in terms of tensor diagrams as

tr$[lr]$ is the inner product of l and r (interpreted as vectors); as normalization convention, we rescale l and r such that their inner product is 1.

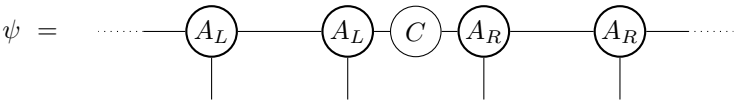
(c) One can show that l is a positive matrix, and thus perform a Cholesky decomposition: $l = L^\dagger L$, where L is an upper right triangular matrix.

As in (a) define new tensors via $(A_L)_{s,:,:} = LA_{s,:,:}L^{-1}$ for all s. Then A_L is left-orthonormal, since



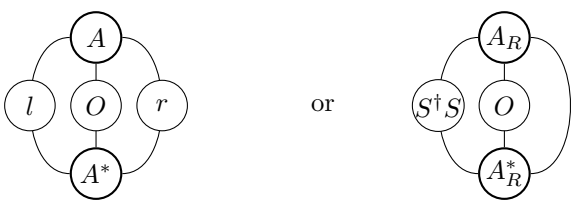
where we have used the eigenvector relation for l. We proceed analogously for r, and corresponding right-orthonormal tensors A_R.

By expressing all tensors A on the left half by A_L, and the remaining tensors on the right half by A_R, one obtains



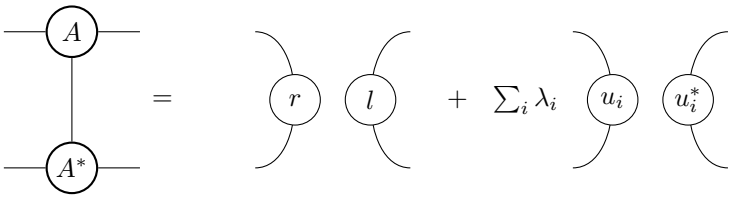
where $C = LR$ originates from a pair of dangling L and R matrices. Finally, we perform a singular value decomposition $C = USV^\dagger$ and absorb U into A_L and $V^\dagger$ into A_R (which does not affect their orthonormalization properties), to arrive at the above bond-canonical form.

(d) When contracting an MPS in uniform or mixed gauge form, any site adjacent to the edge tensors without an observable become the identity matrix or the l or r matrices. Thus, the problem simplifies to



We see that while both forms are easily contractable, the mixed gauge form offers further possibility for optimization as S is a diagonal matrix.

(e) The transfer matrix E (which is a "completely positive" map) admits a spectral decomposition of the following form:



where the λ_i are the eigenvalues smaller than 1 (in absolute value).

The matrix power E^{k-1} can be obtained by raising the eigenalues of E to the power $k-1$, and thus the correlation function simplifies to