Introduction to Basic Density-Matrix Renormalization Group Calculations

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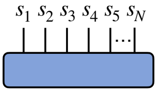
Quantum many-body wavefunctions:

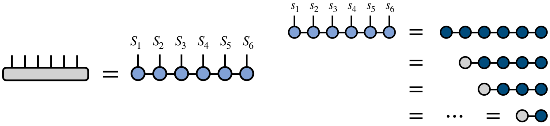
$$|\Psi\rangle = \sum_{s_1, s_2, s_3, \ldots, s_N} \Psi^{s_1 s_2 s_3 \ldots s_N} |s_1, s_2, s_3, \ldots, s_N\rangle.$$

Amplitudes are big tensors.

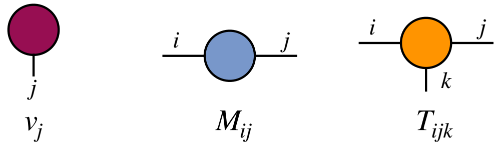
$$\Psi^{s_1 s_2 s_3 s_4 s_5 \ldots s_N} =$$



A matrix product state (MPS) is one of the most widely used tensor network states (area laws of the entanglement entropy, the ground state of gapped/gapless models etc.). Orús, R., Nature Reviews Physics, 1(9), pp.538-550 (2019)



Examples of low-rank tensor:



Tensor Diagram Notations

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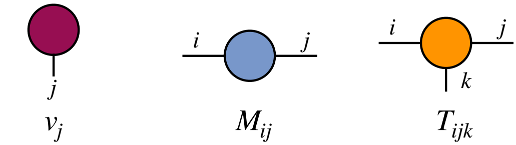
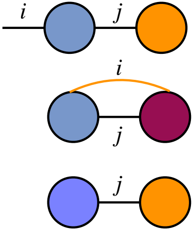


Joining lines implies contraction of indices:



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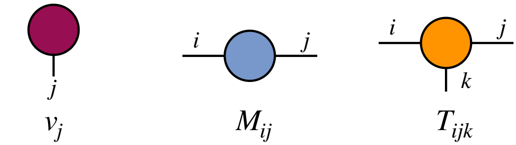

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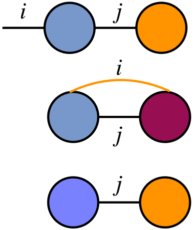
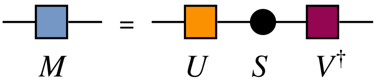


$$\leftrightarrow \sum_j M_{ij} v_j$$

$$\leftrightarrow \sum_{ij} A_{ij} B_{ji} = Tr[AB]$$

$$\leftrightarrow \sum_j w_j v_j$$

Uncover the low-rank structure using singular value decomposition (SVD):



For an arbitrary $m \times n$ matrix M, there exists the singular value decomposition (SVD) with $\ell = min(m, n)$,

$$M = USV^\dagger,$$

where

U is $m \times \ell$ matrix with orthonormal columns ($U^\dagger U = I$),

S is a $\ell \times \ell$ diagonal matrix with non-negative real numbers,

V is a $\ell \times n$ matrix with orthonormal rows ($VV^\dagger = I$).

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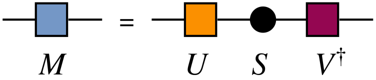
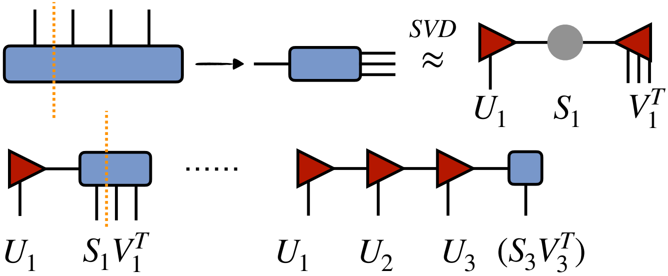


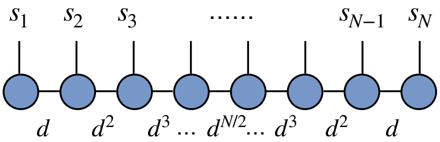
SVD the amplitude tensor sequentially. Using a four-site system as an example.



Goal: reduce dimensionality of $M^{s_{\ell+1}}$

$$|\Psi\rangle = \sum_{\{s\}} A^{s_1} A^{s_2} \dots A^{s_\ell} M^{s_{\ell+1}} B^{s_{\ell+2}} \dots B^{s_N} |s_1, s_2, \dots s_\ell, s_{\ell+1}, s_{\ell+2} \dots, s_N\rangle.$$

Perform SVD on $M^{\ell+1}_{a_\ell, a_{\ell+1}} \to M = U \Lambda V^\dagger$:



$$|\Psi\rangle = \sum_{a_\ell} \lambda_{a_\ell} |a_\ell\rangle_A \cdot |a_\ell\rangle_B$$

with $|a_\ell\rangle_A = \sum_{s_1, s_2, \dots, s_\ell} (A^{s_1} \dots A^{s_\ell})_{1, a_\ell} |s_1, s_2, \dots, s_\ell\rangle$, $(A^{s_\ell} \leftarrow A^{s_\ell} U)$ and $|a_\ell\rangle_B = \sum_{s_{\ell+1} \dots s_N} (B^{s_{\ell+1}} \dots B^{s_N})_{a_\ell, 1} |s_{\ell+1}, \dots s_N\rangle$, $\left(B^{s_\ell+1}_{a_\ell, a_{\ell+1}} = V^\dagger_{a_\ell, s_{\ell+1} a_{\ell+1}}\right)$. Schmidt Decomposition.

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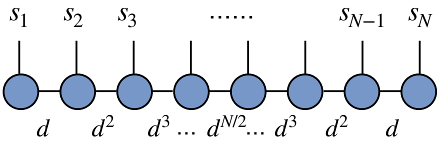
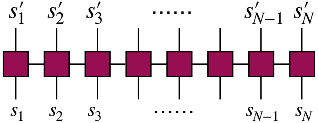


$$|\Psi\rangle = \sum_{a_\ell} \lambda_{a_\ell} |a_\ell\rangle_A \cdot |a_\ell\rangle_B.$$

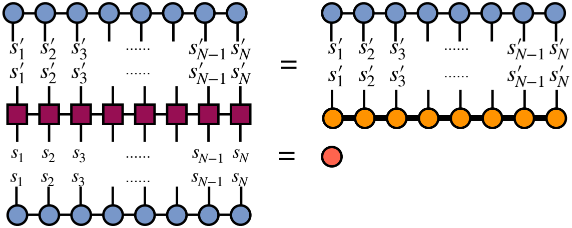
Discard the smallest singular values λ_n such that the *truncation error* is less than ϵ: $\frac{\sum_{n \in discarded} \lambda_n^2}{\sum_n \lambda_n^2} < \epsilon$.

Introduce matrix product operator (MPO) as a generalization of MPS

$$\hat{\mathcal{O}} = \sum_{s}\sum_{s'} M^{s_1,s_1'} M^{s_2,s_2'} \ldots M^{s_N,s_N'} |s_1,\ldots s_N\rangle\langle s_1',\ldots,s_N'|.$$

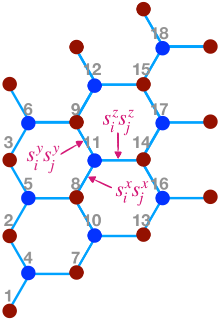


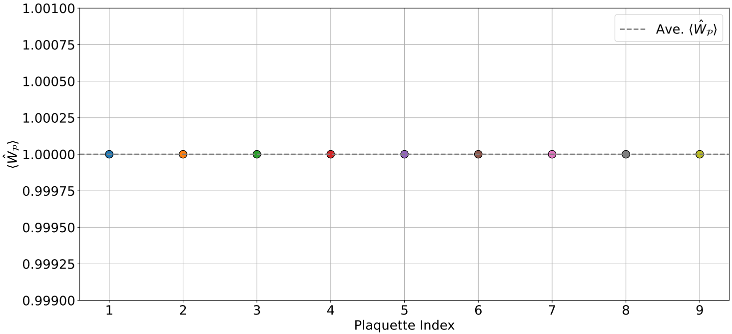
Compute the expectation value $\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle$. U. Schollwöck, "16 DMRG: Ground States, Time Evolution, and Spectral Functions." Emergent Phenomena in Correlated Matter (2013).



The ferromagnetic Kitaev (FMK) on a three-by-three honeycomb lattice,

$$H = -J_x \sum_{\langle i,j \rangle_x} s_i^x s_j^x - J_y \sum_{\langle i,j \rangle_y} s_i^y s_j^y - J_z \sum_{\langle i,j \rangle_z} s_i^z s_j^z .$$





Compute the eigenvalues of plaquette operators on a honeycomb lattice with $N = 2 \times 3 \times 3$ lattice. Use PBC used in both directions. $J_x = 1,\ J_y = 1,\ J_z = 1$.

Assume we have an initial state $|\psi(0)\rangle$, at time t we have

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle.$$

Use the Heisenberg Hamiltonian as an example:

$$H = \sum_{j=1}^{N-1} \left(s_j^z s_{j+1}^z + \frac{1}{2} s_j^+ s_{j+1}^- + \frac{1}{2} s_j^- s_{j+1}^+ \right).$$

Let's Trotterize the time evolution operator $U(t) = e^{-iHt}$:

$$e^{-i\tau H} \approx e^{-ih_{1,2}\tau/2} e^{-ih_{2,3}\tau/2} \dots e^{-ih_{N-1,N}\tau/2} e^{-ih_{N-1,N}\tau/2} \dots e^{-ih_{2,3}\tau/2} e^{-ih_{1,2}\tau/2} + \mathcal{O}(\tau^3)$$

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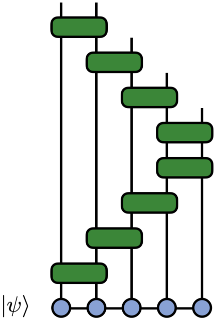
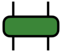




$= e^{-i\tau h_{j,j+1}/2}$

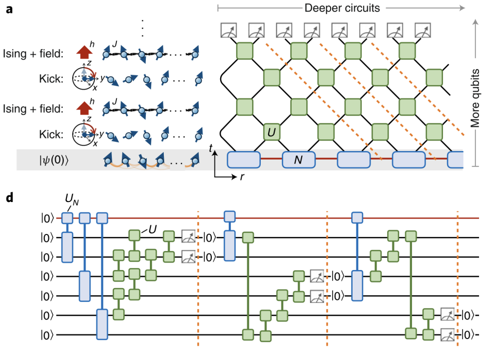
$$h_{j,j+1} = S^z_j S^z_{j+1} + \frac{1}{2} S^+_j S^-_{j+1} + \frac{1}{2} S^-_j S^+_{j+1}$$

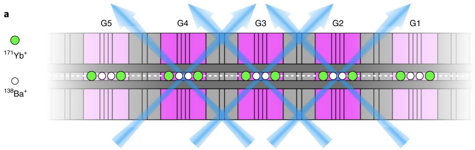
https://itensor.github.io/ITensors.jl/dev/tutorials/MPSTimeEvolution.html

Time-dependent simulations hit an exponential wall after sometime: entanglement increases and $S = \ln \chi$ where χ is the bond dimension.

The Kicked Ising Model

$$H(t) = \sum_i \left(\frac{\pi}{8}\sigma_i^z\sigma_{i+1}^z + h\sigma_i^z + \frac{\pi}{4}\sum_{n\in\mathbb{Z}}\delta(t-n)\sigma_i^x \right).$$





- Mid-circuit measurements and reset.
- Using finite number of qubits to simulate a half-infinite chain.
- E. Chertkov, et al., Nature Physics 18, no. 9 (2022): 1074-1079, I. Kim, preprint arXiv:1702.02093, etc.

The best MPS approximation to the ground state is given by a variational minimization:

$$\min \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \Leftrightarrow \min \left(\langle\Psi|\hat{H}|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle\right)$$

where λ is a Lagrangian multiplier that will give the variational approximation to the ground state energy E_0.

Contract the network to extremize $\langle\Psi|\hat{H}|\Psi\rangle - \lambda\langle\Psi|\Psi\rangle$