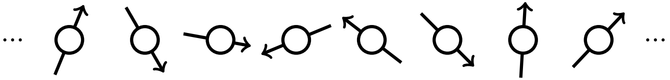
Introduction to Matrix Product States

Jesse Osborne

18 June 2025

Quantum many-body physics

Consider an N-body system:

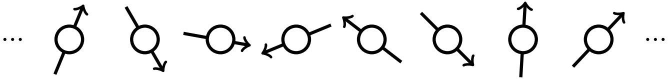


Classical: $\mathcal{O}(N)$ DOFs.

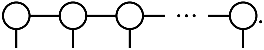
Quantum: $\mathcal{O}(\exp N)$ DOFs.

For classical computers, need to encode important DOFs.

Why matrix product states?



Represent state as a matrix product state (MPS)

$$|\Psi\rangle =$$ 

- Discard ‘long-range’ entanglement, keep local entanglement.
- Good for certain states (area law of entanglement).
- Limited for ‘general’ states (e.g. out of equilibrium).
- Works for 1D or quasi-1D systems.
- Also other varieties of tensor networks.

Singular value decomposition

The fundamental building block of MPS is the

Singular value decomposition (SVD)

For an $n \times m$ matrix M, we can write

$$M = USV^{\dagger},$$

where U and $V^{\dagger}$ are unitary, and S is nonnegative real diagonal (singular value matrix).

- Analogous (but not equivalent) to eigenvalue decomposition.
- Can form an *approximate* SVD by only keeping n largest singular values.

SVD image compression

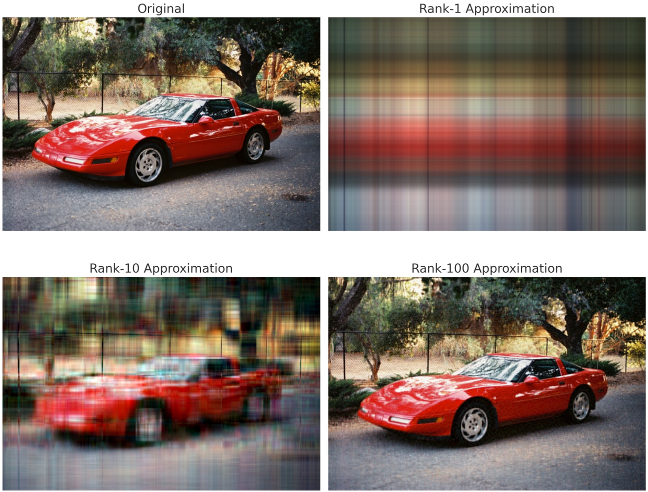


Image taken from Wikipedia: CC BY-SA 4.0 by Samir.beall.
See also: `https://timbaumann.info/svd-image-compression-demo/`

Schmidt decomposition

Given a pure state for an N-body system

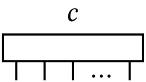
$$\left|\Psi\right\rangle = \sum_{s_1 s_2 \cdots s_N} c^{s_1 s_2 \cdots s_N} \left|s_1\right\rangle \otimes \left|s_2\right\rangle \otimes \cdots \otimes \left|s_N\right\rangle,$$

we make a bipartition between sites n and $n+1$,
view this c as a matrix, and take an SVD

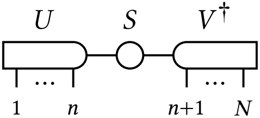
$$c^{(s_1 \cdots s_n)(s_{n+1} \cdots s_N)} = \sum_{ij} U^{(s_1 \cdots s_n) i} S^{ij} (V^\dagger)^{j (s_{n+1} \cdots s_N)}.$$

Schmidt decomposition

Can use graphical notation for tensors:

$|\Psi\rangle =$  .

Taking the Schmidt decomposition:

$|\Psi\rangle =$  .

Entangement entropy $\mathcal{S}$ given in terms of singular values:

$$\mathcal{S} = -\operatorname{Tr}(\rho_A \ln \rho_A) = -\sum_i S_i^2 \ln S_i^2;$$

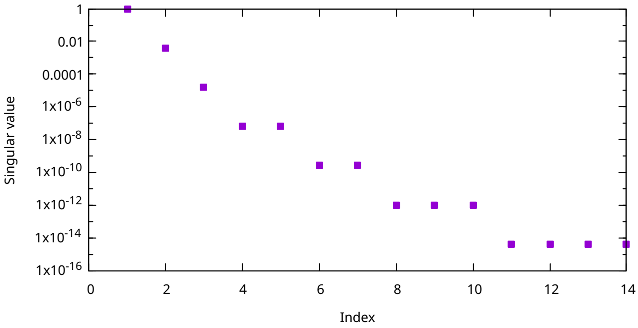
Can we use an approximate SVD here?

Singular value spectrum

Transverse field Ising chain

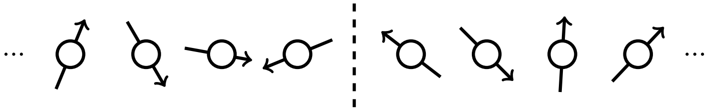
$$\hat{H} = -J \sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + h \sum_j \hat{\sigma}_j^x .$$

Ground state at $h/J = 0.8$:



Spectrum collapses at critical point $h/J = 1$.

Area law of entanglement entropy

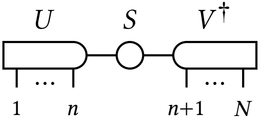


Area law

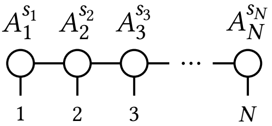
For ground states of local Hamiltonians with an energy gap in *one* spatial dimension, the entanglement entropy of the ground state scales as the *boundary area* of the bipartition (i.e. constant).

- Only need a *constant* number of singular values as $N \to \infty$.
- Critical (gapless) states: area law plus logarithmic correction.
- Holds in some $\geq$ 2D systems (less rigorous proofs).
- Entropy grows (linearly) out of equilibrium.

Matrix product states

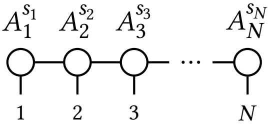
$|\Psi\rangle =$ 

Take a Schmidt decomposition between every pair of sites:

$|\Psi\rangle =$  ,

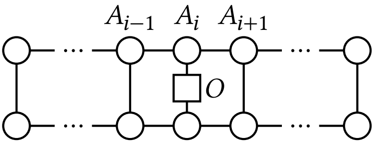
obtain a matrix product state (MPS).

In general, each $A_n^{s_n}$ is a $D \times D$ matrix (D: bond dimension).

$|\Psi\rangle =$ 

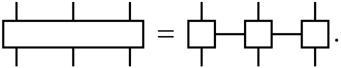
Efficient compression of state: $O(ND^2)$ degrees of freedom (compare $O(\exp N)$ for an arbitrary state).

Efficient evaluation of expectation values:

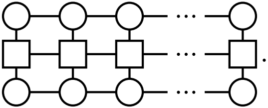
$\langle\Psi|O_i|\Psi\rangle =$  .

Matrix product operators

Decompose larger operators as matrix product operators (MPOs):



Efficiently evaluate global operators, e.g. Hamiltonian:

$\langle \Psi | \hat{H} | \Psi \rangle =$ 

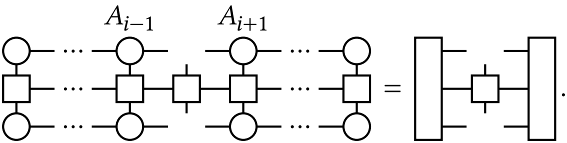
What can we do with MPSs?

- Cannot fully diagonalize Hamiltonian.
- Can find ground states (DMRG).
- Can perform time evolution (limited timescale: entanglement).
- Can look at some excited/thermal states.

To find ground state: minimize energy.

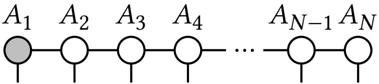
Cannot update entire MPS at once: update tensors one at a time.

To optimize tensor A_i, want to minimize

$\mathscr{H}^i_{\text{eff}} =$ 

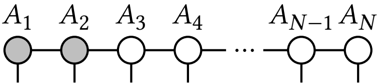
Density matrix renormalization group (DMRG)

Update tensors, sweeping from left to right:



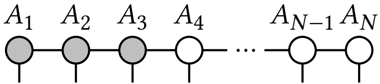
Density matrix renormalization group (DMRG)

Update tensors, sweeping from left to right:



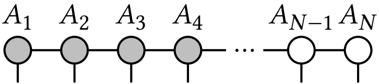
Density matrix renormalization group (DMRG)

Update tensors, sweeping from left to right:



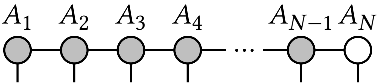
Density matrix renormalization group (DMRG)

Update tensors, sweeping from left to right:



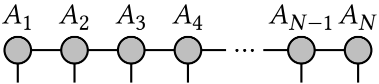
Density matrix renormalization group (DMRG)

Update tensors, sweeping from left to right:



Density matrix renormalization group (DMRG)

Update tensors, sweeping from left to right:



Sample Python DMRG code

`https://mptoolkit.qusim.net/Tutorials/MPS-DMRG`

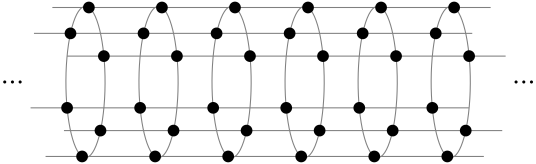
Outlook: Time evolution

$$|\Psi(t + \Delta t)\rangle = \mathrm{e}^{\mathrm{i}\hat{H}\Delta t} |\Psi(t)\rangle$$

- Can replace energy optimization in DMRG with time propagation (time-dependent variational principle: TDVP).
- Can approximate the time-evolution operator (time-evolving block decimation: TEBD; MPO time evolution).

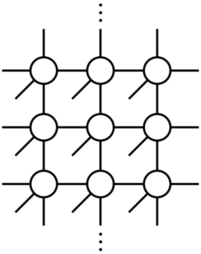
Outlook: Other directions

- Infinite states by explicitly enforcing translation invariance.
- Explicitly enforce global symmetries by writing tensors in quantum number blocks.
- Can look at two-dimensional systems by using cylinders:



Exponential growth in bond dimension with circumference.

Other types of *tensor networks* for higher spatial dimensions:

$|\Psi\rangle = \cdots$  $\cdots .$

Downside: Less efficient algorithms compared with MPS.

Further reading

U. Schollwöck, *The density-matrix renormalization group in the age of matrix product states*, Annals of Physics **326**, 96 (2011).

J. C. Bridgeman and C. T. Chubb, *Hand-waving and interpretive dance: an introductory course on tensor networks*, Journal of Physics A: Mathematical and Theoretical **50**, 223001 (2017).