Matrix Product States

Atithi Acharya

December 14, 2020

Outline

- What is an MPS?
- Which quantum states can be approximated well by MPS?
  - Area law of entanglement entropy
  - Gapped systems
- Tensor network diagrams
- Examples (exact MPS)
  - AKLT state
  - GHZ state
- Connection between MPS and Hamiltonian
- Ground state of local Hamiltonians as MPS
  Example: Transverse Field Ising Model
- Bottlenecks and limitations

Definition

Quantum system living on N sites. $\{s_i\}$ where $i \in \{1, 2..., N\}$
Example: spin-$\frac{1}{2}$, $d = 2$ (d-local)
Hilbert space:

$$\mathcal{H} = \otimes_{i=1}^{N} \mathcal{H}_i \quad \mathcal{H}_i = \{|1_i\rangle \dots |d_i\rangle\}$$

Most general state (not necessarily 1D):

$$|\psi\rangle = \sum_{1,\dots,s_N} c^{s_1 \dots s_N} |s_1, \dots, s_N\rangle$$

When the $c^{s_1 \dots s_N}$ factorizes (mean-field approx), we use conditions such as

$$c^{s_1 \dots s_N} = c^{s_1} c^{s_2} .. c^{s_N}$$

But this won't allow us to capture entanglement. **Need Generalization !**

Matrix Product State

Generalize to matrices,

$$c^{s_1 \dots s_N} = A^{s_1} A^{s_2} .. A^{s_N}$$

$$|\Psi\rangle = \sum_{\{s\}} \mathrm{Tr}[A^{s_1} A^{s_2} \dots A^{s_N}] |s_1 s_2 \dots s_N\rangle$$

$A_i^{s_i}$ are complex-square matrices of order χ and s_i are spin indices for site i.
For a d-level system, $s_i \in \{0, 1 ..., d-1\})$.

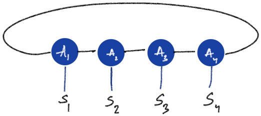


Figure: Roger Penrose graphical notation of tensors:

Question

When can we find a small enough i.e. practical bond dimension χ??

Entanglement

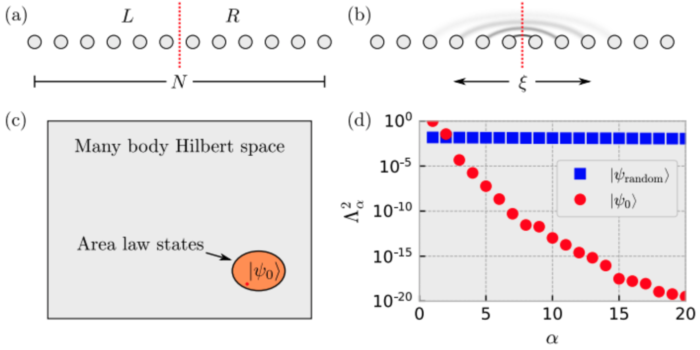


Figure: (a): Bipartition of a 1D system. (b): Significant quantum fluctuations within correlation length. (c) In the many body Hilbert space, area law states lie in a corner but they include all gapped ground states. (d) Largest Schmidt values of the ground state of the TFIM. Reference [1]

[1] Efficient TeNPy numerical simulations by Frank Pollman 2018

Entanglement

- Schmidt decomposition of a pure state $|\Psi\rangle \in \mathcal{H}$ where $\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_R$

$$|\Psi\rangle = \sum_{\alpha} \Lambda_\alpha \, |\alpha\rangle_L \otimes |\alpha\rangle_R$$

- The reduced density matrix $\rho^R = Tr_L(|\psi\rangle\langle\psi|)$
- Von-Neumann entropy is given as

$$S = -Tr(\rho^R log(\rho^R))$$

- Since $\rho^R = \sum_\alpha \Lambda_\alpha^2 \, |\alpha\rangle_R \, \langle\alpha|_R$,

$$S = -Tr(\Lambda_\alpha^2 log(\Lambda_\alpha^2))$$

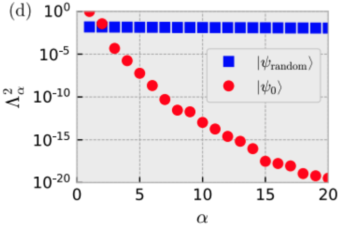


Figure: Decaying Schmidt values for Tranverse Field Ising model. The entanglement spectrum in terms of Schmidt values i.e spectrum of reduced density matrix $\Lambda_\alpha^2 = exp(-\epsilon_\alpha)$ for each α. **The decay in $|\psi_0\rangle$ guarantees existence of an MPS representation with low enough χ**

Volume law vs Area law

Volume law: In a system of N sites with on-site Hilbert space dimension d (e.g. $d = 2$), for a bipartition into two $N/2$ sites, a randomly drawn ("typical") state $|\psi_{random}\rangle$ has EE of of the order

$$S(N) \sim \frac{N}{2} log(d)$$

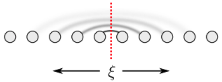
Why log(d)??: Completely mixed state locally yields

$$S = -\sum_{0}^{d-1} \frac{1}{d} log(1/d) = log(d)$$

Volume law vs Area law

Area law: In contrast, if we are looking at ground states $|\psi_0\rangle$ of gapped and local Hamiltonians, it follows area law of entanglement scaling i.e. $S(N)$ is **constant** for $N > \xi$ where ξ is the correlation length.

Why: A gapped state contains fluctuations within the correlation length ξ and thus only degree of freedoms near the cut are entangled.



Given a gapped local 1D Hamiltonian, its ground state is well approximated by an MPS. M.B. Hastings 2006 [1] (Why: Since it can be shown that gapped Hamiltonians will have area law entanglement entropy scaling).

Gapped Systems

Definition

When the system size $N \to \infty$, the Hamiltonian H is gapped if one of the following is true.

- The ground state degeneracy m_N of H_N is upper bounded by finite integer m and the gap between the ground states and the first excited states of H_N is lower bounded by a finite positive number Δ
- There are finite number m of lowest energy states which have energy separations exponentially small in N. And the separation of these states to all other states is lower bounded by finite number Δ for arbitrary N.

Examples: AKLT state

- The AKLT (Affleck,Lieb,Kennedy and Tasaki) Hamiltonian,

$$H = J\sum_{i=0}^{N-1}\left(\frac{1}{3}+\frac{1}{2}S^{(i)}\cdot S^{(i+1)}+\frac{1}{6}(S^{(i)}\cdot S^{(i+1)})^2\right) \tag{1}$$

- The matrix product state of the AKLT ground state which has a bond dimension of $\chi = 2$ can be written as (4) using

$$A^{+} = \sqrt{\frac{2}{3}}\sigma^{+}, A^{0} = \frac{-1}{\sqrt{3}}\sigma^{z}, A^{-} = -\sqrt{\frac{2}{3}}\sigma^{-} \tag{2}$$

- Reminder:

$$|\Psi\rangle = \sum_{\{s\}}\mathrm{Tr}[A^{s_1}A^{s_2}\dots A^{s_N}]|s_1 s_2 \dots s_N\rangle$$

Tensor network diagrams

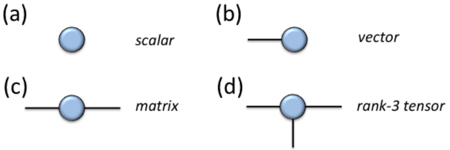


Figure: Tensor network diagrams: (a) scalar, (b) vector, (c) matrix and (d) rank-3 tensor. Introduction to tensor networks by Roman Orus [2].

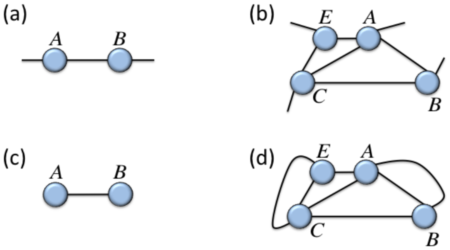


Figure: (a) matrix product, (b) contraction of 4 tensors with 4 open indices, (c) scalar product of vectors, and (d) contraction of 4 tensors without open indices

Matrix Product AKLT state

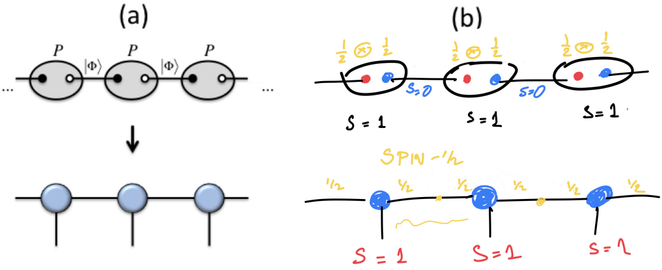
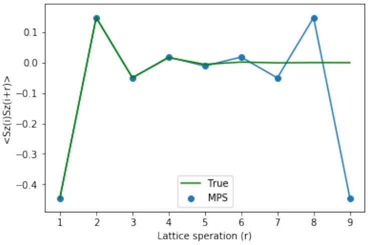
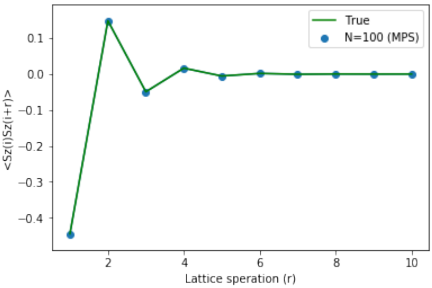


Figure: MPS for the AKLT state: (a) spin-1/2 particles arranged in singlets $|\Phi\rangle = 2^{-1/2}(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle)$, and projected [2]by pairs into the spin-1 subspace by projector P; (b) In the MPS description, the spin-1/2's live on the bonds.

Correlations in AKLT state



(a) Correlation function for small system sizes (N=10)



(b) Correlation function for N=100

Figure: True correlation function $\langle S_z^{(i)} S_z^{(i+r)} \rangle \propto \left(\frac{-1}{3}\right)^r$ (as a function of r). With periodic b.c. the plots for ground states not coincide with that of the analytical expression very well. Subplot (b): We use $N = 100$ and plot the first 10 correlations.

Example: GHZ State

- The Greenberger Horne Zeilinger (GHZ) state is a highly entangled quantum state of $N > 2$ subsystems and is often used to investigate multiparticle entanglement [3]. The correlations present in this state are heavily utilized in many quantum information tasks such as quantum cryptography.
- The GHZ state of N spins-1/2 is given by

$$|\Psi_{GHZ}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle^{\otimes N} + |1\rangle^{\otimes N}\right) \tag{3}$$

- Represented exactly by a MPS with bond dimension $\chi = 2$ and periodic boundary conditions. The A matrices upto normalization can be written as

$$.A^{+} = 1 + \sigma_z, A^{-} = 1 - \sigma_z \tag{4}$$

where $|0\rangle$ and $|1\rangle$ are e.g. the eigenstates of the Pauli σ_z operator.

GHZ state

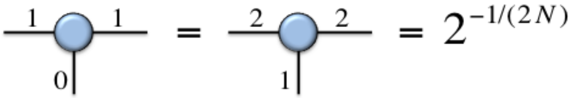


Figure: Non-zero components for the MPS tensors of the GHZ state. This figure is from introduction to tensor networks by Roman Orus [2].

The MPS representation for GHZ is also nicely visualized using tensor notations in matrices.

$$A = \begin{bmatrix} |0\rangle & 0 \\ 0 & |1\rangle \end{bmatrix}, \quad AA = \begin{bmatrix} |00\rangle & 0 \\ 0 & |11\rangle \end{bmatrix}, \quad AAA = \begin{bmatrix} |000\rangle & 0 \\ 0 & |111\rangle \end{bmatrix} \tag{5}$$

Singular Value Decomposition (SVD)

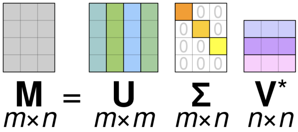
$$M = USV^{\dagger}$$

$$U \quad dim.(m \times k) \quad U^{\dagger}U = I$$

$$S \quad dim.(k \times k) \quad \mathrm{k} = \min(\mathrm{n}, \mathrm{m})$$

Non-vanishing singular values rank $r \leq k$.

$$V^{\dagger} \quad dim.(k \times n) \quad V^{\dagger}V = I \quad (row)$$



Obtaining the A matrices

- (a) Rewriting $c_{s_1 \dots s_N} = \Psi_{s_1 \dots s_N}$, $|\psi\rangle = \sum_{1,\dots,s_N} \Psi \, |s_1, \dots, s_N\rangle$
- (b) After 1 SVD,

$$c_{s_1 \dots s_N} = \sum_{a_1}^{r_1} A^{s_1}_{a_1} \Psi_{(a_1 s_2),(s_3..s_N)}$$

The rank $r_1 \leq d$ where d is local dimension.

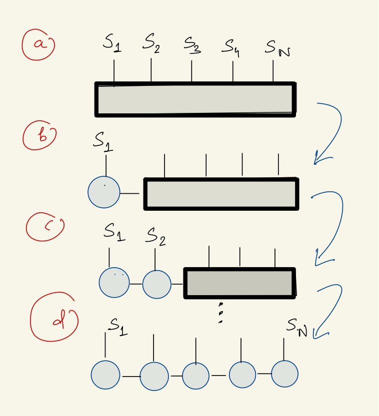


Figure: Graphical representation of an iterative construction of an exact MPS representation from an arbitary quantum state.

Obtaining the A matrices

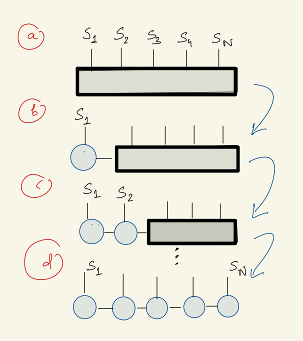
- (c) After 2 SVDs,

$$c_{s_1 \dots s_N} = \sum_{a_1}^{r_1} \sum_{a_2}^{r_2} A_{a_1}^{s_1} A_{a_1,a_2}^{s_2} \Psi_{(a_2 s_1),(s_3..s_N)}$$

- (d) Finally after further SVDs each successively on smaller matrices, we get

$$c_{s_1 \dots s_N} = \sum_{a_1,a_2..a^N}^{r_1,r_2..,r_N} A_{a_1}^{s_1} A_{a_1,a_2}^{s_2} A_{a_2,a_3}^{s_3} \dots A_{a_{N-1}}^{s_N}$$

- $A_{a_1}^{s_1}$ and $A_{a_{N-1}}^{s_N}$ are vectors. We have obtained a matrix product state (evident from the contracted indices $(a_2, a_3.., a_{a_{N-2}})$



Connection between MPS and Hamiltonian

There are two directions to draw connections.

- Given an MPS, what can we tell about its parent Hamiltonian?
- Given a Hamiltonian with additional properties, what can we tell about the MPS approxmiation of its ground state or the existence of an exact MPS representation for its ground state.

Summary of connection

Here is a very short summary of the two connections.

- For every MPS, it can be shown that it naturally appears from a frustration free [3]local parent Hamiltonian.
- Given a gapped local 1D Hamiltonian, its ground state is well approximated by an MPS. M.B. Hastings [1] (Why: Since it can be shown that gapped Hamiltonians will have area law entanglement entropy scaling).

[3]A local Hamiltonian, $H = \sum_j H_j$ is frustration free when its ground state energy $E_0 = \sum_j E_{0j}$

Direction of proofs

For any arbitrary MPS, it can be shown that it naturally appears from a gapped, local and frustration free [4]parent Hamiltonian. What about its converse?

- If we construct a local, gapped Hamiltonian and **not frustration free**, does that guarantee the groundstate will not be an exact MPS ??
- Moreover, the proof given by Hastings (2006,2007) [5]holds rigorously in one direction. So all we can conclude for the converse, is "**typical**" gapless Hamiltonians will not have MPS ground states.

[5] M.B. hastings. Solving gapped Hamiltonians locally. Physical Review B.73(8), Feb 2006

Ground state of Hamiltonians

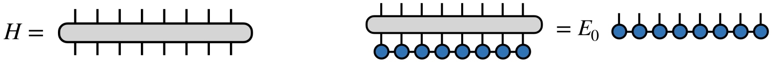
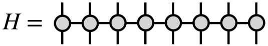


Figure: A Hermitian matrix acting in vector space that is the tensor product of smaller spaces, each of dimension d.
Representing the state as a MPS, we get back eigenvalue when the matrix is contracted with the state.
Our goal is to find the lowest eigenvalue E_0 that corresponds to the ground state.

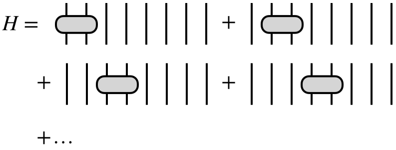
DMRG

The success of density matrix renormalization group is related to the fact that it acts within the space of matrix product states (MPS ansatz) and variationally finds the lowest energy state. Invented in 1992 by Steven R. White.

H as MPO



(a) Matrix Product Operator (MPO)



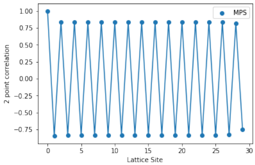
(b) Local structure

Figure: H as a MPO tensor network (this could be very general unless we put restrictions on the bond dimension being small).
Added properties such as locality can be extremely useful in finding the lowest eigenstate efficiently.
For instance, the Hamiltonian corresponding to TFIM is also local. In the right subplot (b) We represent the H as sum of local terms.

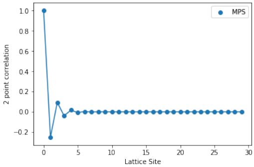
What do we gain from the structure?

- Whenever the interaction is local i.e. it acts non-trivially on some small number of neighbouring sites, if the Hamiltonian is also frustration free i.e. the minimization of energy can be local ($E_{min} = E_{1min} + E_{2min} + ..$) we can find an exact MPS representation of the ground state.
- However, in general we can find MPS approximations to the ground state of the corresponding Hamiltonians.

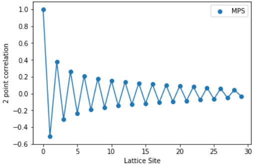
Example: TFIM



(a) $J > h$, $J = 1$ and $h = 0.5$



(b) $J < h$, $J = 1$ and $h = 2.0$



(c) $J = h = 1$

Figure: 2 point functions $\langle \sigma_0^z \sigma_i^z \rangle$ for ground states of antiferromagnetic 1D tranverse field Ising model ($\#$ sites $= 30$) using matrix product states.

$$H = J \sum_{<ij>} \sigma_i^z \sigma_j^z + h \sum_i \sigma^x$$

(a) Long range order since correlations saturates with increasing lattice separation. (b) Exponential decay of the correlations.
(c) At the critical point i.e. $h/J = 1$, polynomial decay in correlations.

Bottlenecks

- **Exponential growth** of bond dimension with system size where exact MPS representations don't exist and a small χ can't be guaranteed.
- The complexity of number of operations (**tensor contractions**) depend on the ordering of indices. Finding the optimal order of indices to be contracted is important. To minimize the computational cost of a contraction one must optimize over the different possible orderings of pairwise contractions, and find the optimal case.
- This issue becomes magnified when we are **no longer** dealing with 1D systems.
- In practice, most of the numerical works in tensor network involve decision of the order of contractions based on inspection.

[1] M. B. Hastings. Solving gapped hamiltonians locally. *Physical Review B*, 73(8), Feb 2006.

[2] Roman Orus. A practical introduction to tensor networks: Matrix product states and projected entangled pair states. *Annals of Physics*, 349:117–158, Oct 2014.

[3] S.B. van Dam, J. Cramer, T.H. Taminiau, and R. Hanson. Multipartite entanglement generation and contextuality tests using nondestructive three-qubit parity measurements. *Physical Review Letters*, 123(5), Jul 2019.