Tensor Networks

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Contents

1 Introduction

Tensor networks are factorizations of very large tensors into networks of smaller tensors, with applications in chemistry, **many body physics**, machine learning, and many other fields.

Many body properties are predicted based on simplified models that are believed to reproduce the relevant interactions responsible for the observed physics, e.g. the Hubbard and $t - J$ models. In a very few lucky cases these models are exactly solvable. Thus we heavily rely on faithful numerical methods to determine many properties especially when we head into curse of dimensionality. Tensor Networks are one example of numerical technique to represent quantum states corresponding to systems who sometime live in exponentially large Hilbert space (e.g. with N spins $1/2$, the dimension of the Hilbert space is 2^N) and compute properties such as expectation values. It is important to note they will work better when we are dealing with relevant states that come out of Hamiltonians with heavy constraints locality i.e. the interactions are local.

There are many members belonging to the family of tensor network states. However, we will look into one member i.e. Matrix Product States (MPS). In our discussion on MPS, we will rely on some of its properties such as the area law scaling of the entanglement entropy in 1d systems. Precisely, it can be shown that the ground states of gapped hamiltonians follow area law entanglement entropy (See article) and thus we can use MPS to represent ground state of such hamiltonians [2] with a gurantee of finite bond dimension (See the section on building blocks for definition). This is in not to be confused with the fact that MPS can represent any quantum state of the many-body Hilbert space just by increasing the value of D sufficiently. There are other members such as MERA (states which has logarithimic corrections to the area law scaling of entanglement entropy) and Projected Entangled Pair states (PEPS). The key difference in PEPS is in its ability to capture polynomially-decaying correlations (critical states) with lattice separation unlike the matrix product states which can at best capture exponentially decaying correlations. [4].

2 Building blocks

2.1 Tensor network diagrams

We see in Fig. (1,2), the schematic representations of tensors and the relationship between tensor contractions and familiar operations such as matrix products (multiplication). The index summed over is now diagrammatically shown as a contraction.

2.2 Tensor Decompositions

This section follows closely from Schollwock [5]

We can study the tensor decomposition of arbitrary quantum states into MPS using either left or right canonical truncation schemes. However, we review only the left truncation scheme here. In left truncation scheme, we reshape the state vector with d^L components into a matrix of dimension $(d \times d^{L-1})$. Then do singular value decompositions, combine terms and after we get rid of the degree of freedoms from left we continue to form matrices for the remaining portion and then SVD until we hit the end where we finally write it as a product of matrices and hence the name Matrix Product States.

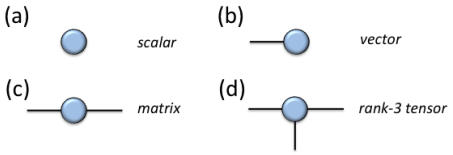


Figure 1: Tensor network diagrams: (a) scalar, (b) vector, (c) matrix and (d) rank-3 tensor. This figure is from introduction to tensor networks by Roman Orus [4].

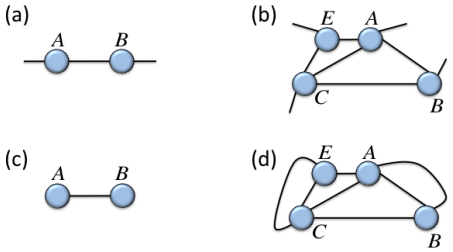


Figure 2: Tensor network diagrams for (a) matrix product, (b) contraction of 4 tensors with 4 open indices, (c) scalar product of vectors, and (d) contraction of 4 tensors without open indices [4]

Consider a lattice of L sites with d-dimensional local state spaces $\{\sigma_i\}$ on sites $i = 1, \ldots, L$. A general pure quantum state ,say on an one-dimensional (not necessarily), can be written as

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1\ldots\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle , \tag{1}$$

where we have exponentially many coefficients $c_{\sigma_1\ldots\sigma_L}$ we *reshape* the state vector with d^L components into a matrix Ψ of dimension $(d \times d^{L-1})$, where the coefficients are related as

$$\Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = c_{\sigma_1\ldots\sigma_L}. \tag{2}$$

An SVD of Ψ gives

$$c_{\sigma_1\ldots\sigma_L} = \Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = \sum_{a_1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} (V^\dagger)_{a_1,(\sigma_2\ldots\sigma_L)} \equiv \sum_{a_1}^{r_1} U_{\sigma_1,a_1} c_{a_1\sigma_2\ldots\sigma_L}, \tag{3}$$

where in the last equality S and $V^\dagger$ have been multiplied and the resulting matrix has been reshaped back into a vector. The rank is $r_1 \leq d$. We now decompose the matrix U into a collection of d row vectors A^{σ_1} with entries $A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1}$. At the same time, we reshape $c_{a_1\sigma_2\ldots\sigma_L}$ into a matrix $\Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}$ of dimension $(r_1 d \times d^{L-2})$, to give

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}. \tag{4}$$

Ψ is subjected to an SVD, and we have

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}, \tag{5}$$

where we have replaced U by a set of d matrices A^{σ_2} of dimension $(r_1 \times r_2)$ with entries $A^{\sigma_2}_{a_1,a_2} = U_{(a_1\sigma_2),a_2}$ and multiplied S and $V^\dagger$, to be reshaped into a matrix Ψ of dimension $(r_2 d \times d^{L-3})$, where $r_2 \leq r_1 d \leq d^2$. Upon further SVDs, we obtain

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1,\ldots,a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \ldots A^{\sigma_{L_1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1}} \tag{6}$$

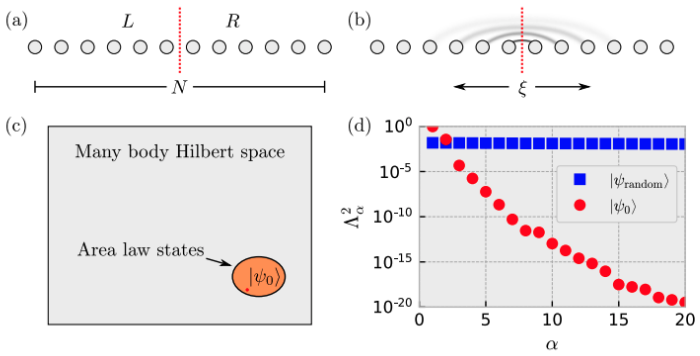


Figure 3: (a): Bipartition of a 1D system. (b): Significant quantum fluctuations within correlation length. (c) In the many body Hilbert space, area law states lie in a corner but they include all gapped ground states. (d) Largest Schmidt values of the ground state of the TFIM. [3]

or more compactly

$$c_{\sigma_1 \ldots \sigma_L} = A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_{L-1}} A^{\sigma_L}, \tag{7}$$

where we have recognized the sums over a_1, a_2 and so forth as matrix multiplications. In any case, the (arbitrary) quantum state is now represented exactly in the form of a *matrix product state:*

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle . \tag{8}$$

3 Which states can be approximated as MPS

3.1 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 $\rho^R = \sum_\alpha \Lambda^2_\alpha |\alpha\rangle_R \langle\alpha|_R$,

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

The decay in Schmidt values for ground state $|\psi_0\rangle$ guarantees existence of an MPS representation with low enough χ. See Fig. (4)

3.2 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

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

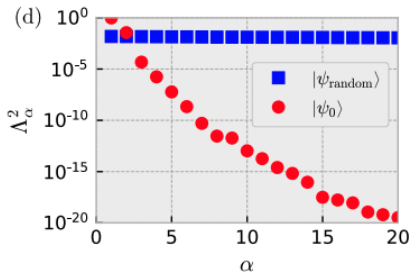


Figure 4: Decaying Schmidt values for Tranverse Field Ising model. The entanglement spectrum in terms of Schmidt values i.e spectrum of reduced density matrix $\Lambda_\alpha^2 = exp(-\epsilon_\alpha)$ for each α. [3]

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

$$S = -\sum_0^{d-1} \frac{1}{d} log(1/d) = log(d)$$

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. Since it can be shown that gapped Hamiltonians will have area law entanglement entropy scaling, given a gapped local 1D Hamiltonian, its ground state is well approximated by an MPS. M.B. Hastings 2006 [2]

Gapped Hamiltonian: 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.

4 Examples of MPS (exact)

$$|\Psi\rangle = \sum_{\{s\}} \text{Tr}[A^{s_1} A^{s_2} \dots A^{s_N}] |s_1 s_2 \dots s_N\rangle \tag{9}$$

4.1 AKLT state

AKLT model (CITATION) named after (Affleck, Lieb, Kennedy and Tasaki) has provided crucial insights into the spin-1 Heisenberg chain since its an exactly solvable model that exhibits "Haldane gap". We use the notation $|+\rangle, |\mathbf{0}\rangle, |-\rangle$ as the spin-1 basis states. The matrix product state of the

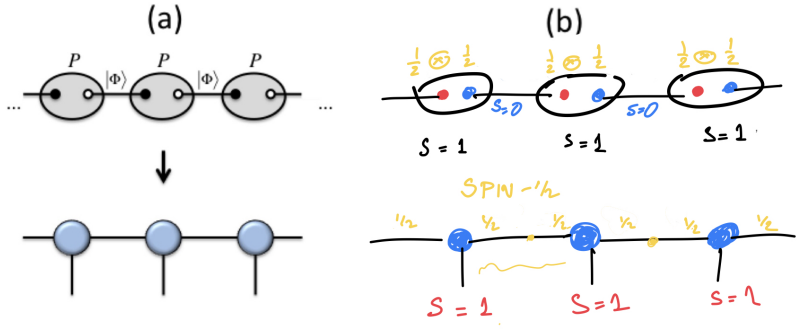


Figure 5: MPS for the AKLT state: (a) spin-$1/2$ particles arranged in singlets $|\Phi\rangle = 2^{-1/2}(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle)$, and projected [1]by pairs into the spin-1 subspace by projector P; (b) In the MPS description, the spin-1/2's live on the bonds.

AKLT ground state which has a bond dimension of $\chi = 2$ can be written as (9) using

$$A^+ = \sqrt{\frac{2}{3}}\sigma^+, A^0 = \frac{-1}{\sqrt{3}}\sigma^z, A^- = -\sqrt{\frac{2}{3}}\sigma^- \tag{11}$$

Since the order of the A matrices (complex square) defines the bond dimension, we clearly see $\chi = 2$. Also, A can be written using the Pauli matrices (a particular gauge choice). We can verify that this annihilates the AKLT Hamiltonian as follows,

$$H = J \sum_{i=0}^{N-1} \left(\frac{1}{3} + \frac{1}{2} S^{(i)} \cdot S^{(i+1)} + \frac{1}{6} (S^{(i)} \cdot S^{(i+1)})^2 \right) \tag{12}$$

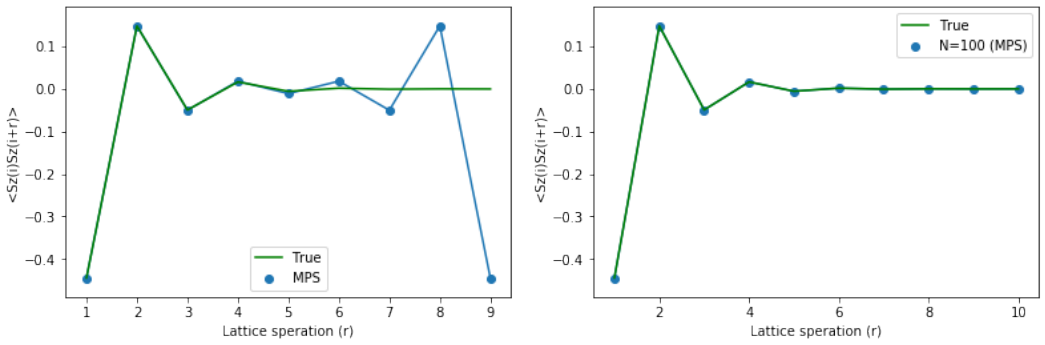
We use the periodic boundary conditions (write-up and code), where the N^{th} spin is identified with 0^{th} spin. $S^{(i)}$ denotes the vector of spin sperators $(S_x^{(i)}, S_y^{(i)}, S_z^{(i)})$. We can always verify the reconstruction using matrix product states by directly computing L^1 or L^2 norm between the exact eigenstates and the MPS reconstruction. This could be extended to the Frobenius norm [2]between matrix product operators (MPOs). However, obtaining the state itself is limited with curse of dimensionality and thus we have to verify the reconstruction of the states by computing other relevant quantities such as correlation functions. For instance, we know theoretically that the Z-Z correlations of the ground state corresponding to the AKLT Hamiltonian (12) scales exponentially as a function of r i.e. $(\left(\frac{-1}{3}\right)^r)$ where $r = |i - j|$. See Fig. (6)

[1]The projectors mentioned in Fig.5 can be written as

$$P = |+\rangle\langle 11| + \frac{1}{\sqrt{2}} |\mathbf{0}\rangle \left(\langle 01| + \langle 10|\right) + |\text{-}\rangle\langle 00| \tag{10}$$

[2]Frobenius norm:$\|A\|_{\mathrm{F}} = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2} = \sqrt{\mathrm{trace}\,(A^* A)}$

$$\|A - B\|_{\mathrm{F}} = \sqrt{\mathrm{trace}\,((A-B)^*(A-B))}$$



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

(b) Correlation function for N=100

Figure 6: True correlation function $\langle S_z^{(i)} S_z^{(i+r)} \rangle \propto \left(\frac{-1}{3}\right)^r$ (as a function of r). We see that with periodic boundary conditions the plots for ground states obtained using MPS representation do not coincide with that of the analytical expression very well. Although, with exact diagonalization techiniques we can't scale up the system sizes to in fact observe agreement with the $N \to \infty$ limit, we can do it with matrix product states. See the subplot (b) to the right where we use $N = 100$ and plot the first 10 correlations. The codes for these plots can can be found here.

4.2 GHZ

The Greenberger Horne Zeilinger (GHZ) state is a highly entangled quantum state of $N > 2$ subsystems and is often used to investigate multiparticle entanglement [6]. The GHZ state of N spins-$1/2$ is given by

$$|\Psi_{GHZ}\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle^{\otimes N} + |1\rangle^{\otimes N}\right) \tag{13}$$

where $|0\rangle$ and $|1\rangle$ are e.g. the eigenstates of the Pauli σ_z operator. This is a highly entangled quantum state of the N spins, which has some non-trivial entanglement properties (e.g. it violates certain N-partite Bell inequalities). Still, this state can be represented exactly by a MPS with bond dimension $\chi = 2$ and periodic boundary conditions. The A matrices upto normalization can be written as

$$.A^+ = \mathbb{1} + \sigma_z, A^- = \mathbb{1} - \sigma_z \tag{14}$$

The non-zero coefficients in the tensor are shown in the diagram of Fig.(7). The 3-qubit GHZ state is the simplest one $|\Psi_{GHZ}\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$. The correlations present in this state are heavily utilized in many quantum information tasks such as quantum cryptography. Simple quantum circuits exist which create this state. It is a natural extension of a circuit designed to create Bell states (i.e. $|\Psi_{Bell}\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$).

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

$$A = \begin{bmatrix} |0\rangle & 0 \\ 0 & |1\rangle \end{bmatrix}, \quad AA = \begin{bmatrix} |00\rangle & 0 \\ 0 & |11\rangle \end{bmatrix}, \quad AAA = \begin{bmatrix} |000\rangle & 0 \\ 0 & |111\rangle \end{bmatrix} \tag{15}$$

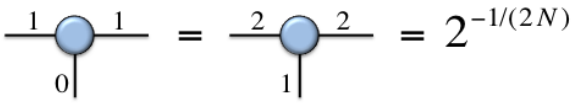


Figure 7: Non-zero components for the MPS tensors of the GHZ state. This figure is from introduction to tensor networks by Roman Orus [4].

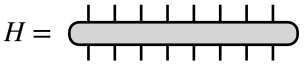


Figure 8: A Hermitian matrix H

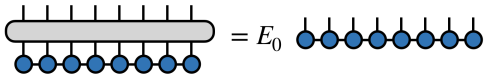


Figure 9: A Hermitian matrix acting in vector space that is the tensor product of smaller spaces, each of dimension d. Representing the state as a MPS, we get back eigenvalue when the matrix is contracted with the state. Our goal is to find the lowest eigenvalue E_0 that corresponds to the ground state.

Thus taking trace of these product of matrices we do get the GHZ state. For instance, $trace(AA) = |00\rangle + |11\rangle$ i.e. the two qubit GHZ state upto a normalization. Simple verification has been numerically done in the code shared [1].

4.3 Obtaining the A matrices

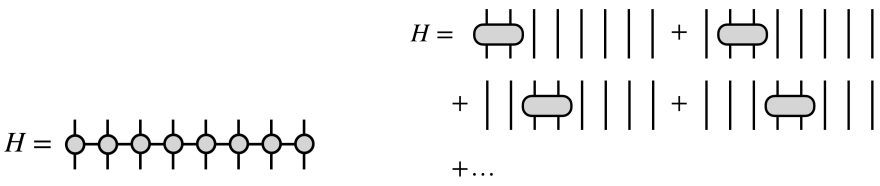
Following the tensor decomposition schemes 2.2, we can show explicit computations of the A matrices corresponding to both GHZ and AKLT. Main motivation here is to again diagrammatically show the scheme presented in 2.2.

5 Ground state properties using tensor networks

The general idea is well explained in [5]. The idea of variationally computing the lowest-energy matrix product state wavefunction of a Hamiltonian was introduced by Dr. Steve White and is known as DMRG (density matrix renormalization group [7]). We can specifically look into the use case in models such as Transverse Field Ising model and 1D Heisenberg spin chains (with and without disorder).

5.1 Problem Statement using tensor network

Before diving into the details of the models, it is worthwhile to remind ourselves the problem statement of DMRG algorithm (not the actual steps involved) using tensor network diagrams. See Fig. 10.



(a) MPO (b) Local structure

Figure 10: Properties of H: In general H could be given 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. Loosely speaking, 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.

5.2 Example: 1D Transverse field Ising model

We take antiferromagnetic ($J > 0$ in Eq. (16)) transverse field Ising model in 1D.

$$H = J \sum_{<ij>} \sigma_i^z \sigma_j^z + h \sum_i \sigma^x \tag{16}$$

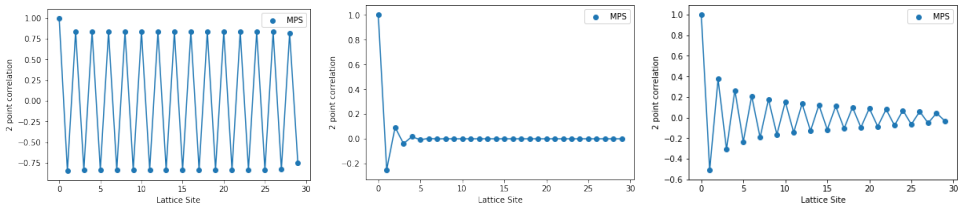
The quantum critical point at $h/J = 1$ will be exhibited by the power-law decay of the correlations. In other regimes, $\sigma_z \sigma_z$ correlations the ground states decay exponentially. We construct the Hamiltonian using matrix product operators and then find the MPS representation of the groundstate. Then include the correlations for the ground state for bigger system sizes of 30 sites (in the plot) where Exact Diagonalization can't be used. Note: This could be extended to much larger system sizes using th formalism. The correlations can be plotted using the matrix product representations of the ground states of the antiferro TFIM in various regimes of parameters i.e. at the quantum critical point, above and below the points.

5.3 Connection between MPS and Hamiltonian

There are two directions

- 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.

Here is a very short summary of the two connections.



(a) $J > h$, $J = 1$ and $h = 0.5$ (b) $J < h$, $J = 1$ and $h = 2.0$ (c) $J = h = 1$

Figure 11: 2 point functions $\langle \sigma_0^z \sigma_i^z \rangle$ for ground states of antiferromagnetic 1D tranverse field Ising model using matrix product states. In the plot to the left, we do see long range order since correlations saturates with increasing lattice separation. In the plot to the right, we see the exponential decay of the correlations.The lattice size is 30.

- 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. [2] (Why: Since it can be shown that gapped Hamiltonians will have area law entanglement entropy scaling).

6 Botttlenecks, limitations, Conclusion

1) Exponential growth of bond dimension where the exact MPS representations don't exist.
2) The complexity of number of operations (tensor contractions) depend on the ordering of indices. In order to use tensor network representations as efficiently as possible, 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 can become intractable and is also a mathematically hard problem to address. Conclusive work is yet to be done addressing this. In practice, most of the numerical works in tensor network involve decision of the order of contractions based on inspection.

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