Introduction to Tensor Networks and 1D spin systems with MERA

Submitted By

Sandeepan Sahoo

School of Physical Sciences

National Institute of Science, Education and Research (NISER), Bhubaneswar

Abstract

Tensor networks are a class of variational wave functions that can be used to study many-body quantum systems. In this report we give a primer on tensor networks by introducing the matrix product state and why such an ansatz is needed to satisfy the Area Law. We then specialize to our core problem and discuss the problems of growth of Hilbert space and rising computational costs involved in rescaling and how it can be resolved using the mulit-scale entanglement renormalization ansatz (MERA). We then present results we have computed for the 1D Ising model for n=16 and n=128 sites.

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Chapter 1

Area Law

For a quantum mechanical system with a state $|\psi\rangle$ and density matrix $\rho = \langle\psi| \, |\psi\rangle$, the Von Neumann entropy is given by

$$S(\rho) = Tr[\rho \ln \rho] \tag{1.1}$$

It gives the measure of how mixed or pure a state is. The Von Neumann entropy of a pure state is zero. For a composite system, i.e. whose Hilbert space is composed of two subsystems A and B, the state can be represented as

$$|\psi\rangle_{AB} = \sum_{ij} c_{ij} \, |i\rangle \, |j\rangle \tag{1.2}$$

The state is separable if $c_{ij} = c_i^A c_j^B$ for all c_{ij}, else it is an entangled state. While its Von Neumann entropy is 0 as a whole, the entropy of the subsystems is positive and give a measure of how entangled they are; hence, entanglement entropy. To measure the entanglement entropy of the system, we define the reduced density matrix

$$\rho_A = \sum_{j}^{N_B} \langle j_B| \, |\psi\rangle \, \langle\psi| \, |j_B\rangle = Tr_B \rho \tag{1.3}$$

It is the partial trace of the density matrix ρ over only the subsystem B. Similarly the reduced density matrix of B would be defined as the trace of ρ over subsystem A. From this the Entanglement entropy

$$S(\rho_A) = Tr[\rho_A ln \rho_A] \tag{1.4}$$

Indeed we can do this for any entangled state. A lattice of L sites and we make a bipartition to separate it into 2 parts A and L-A, The entanglement between such region and the rest of the system is quantified by the Von Neumann. entropy of the reduced density matrix $\rho_A = Tr_{L-A} \, |\psi\rangle \, \langle\psi|$. The maximal value of this entropy will be proportional to $L_A \, \text{lnd}$, L_A being the number of sites in that region A for a d^2 dimensional Hilbert space.

1.1 Area Law

The Area Law states that for any ground state of local noncritical [1] Hamiltonians of the type in Eq. (11.81), the entanglement entropy of a bipartition into regions A and B scales as the boundary of one of the two regions:

$$S(\rho_A) \propto= \partial A \tag{1.5}$$

This has been verified for gapped systems in 1D. However at Quantum criticality, logarithmic corrections may arise, especially for gapless Hamiltonians.

The Area Law can be visualized as the number of bonds required in the dividing the system into 2 parts. For 1D, we can just cut the chain at any site, independent of length. For 2D, we have to cut the bonds across a line and the number of bonds we cut is proportional to the length of that line, hence it grows linearly. For 3D, we have to sweep across a surface and the number of bonds we cut is proportional to the area of that surface.
This has been contrasted with the volume law for the entanglement entropy, which typically occurs for random states or for thermal states in non-equilibirum states. An interesting situation occurs in 1D, where the area-law condition means that the entropy does not scale at all with the size of the region A.

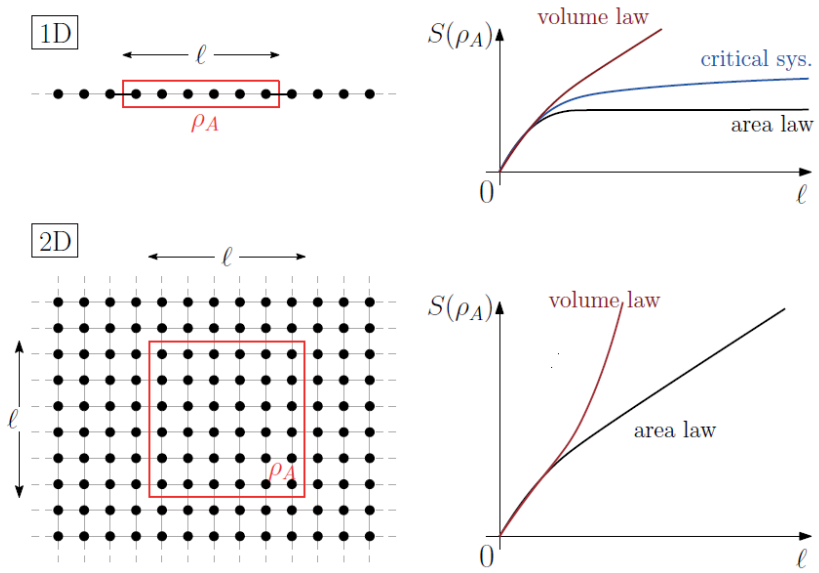

Fig. 1.1: In 1D, the entanglement entropy doesn't scale with l. For critical systems, it should scale as lnl. In 2D, for l^2 sites, it scales as l

1.2 MPS

To build an ansatz that satisfies Area law in 1D, consider a chain of length L and decompose it into 2 subsystems each of which lives on a Hilbert space of dimension χ.
Any state in this Auxilary space can be written as

$$|\psi_{Aux}\rangle = \sum_{\alpha\beta} c_{ij} |\alpha_i\rangle_A |\beta_j\rangle_B \tag{1.6}$$

with i=1,...,L and j=1,...,L. α and β represent a basis corresponding to subsystems A and B, running from 1 to χ at each site.
For the nearest neighbours, i.e. k, k+1, adjacent pairs of these subsystems are then maximally entangled and each pair can be written as

$$|k\rangle = \frac{1}{\chi} \sum_{w=1}^{\chi} |w\rangle_{As} |w'\rangle_{Bs+1} \tag{1.7}$$

Then we can write the global state as

$$|psi\rangle = \otimes_{s=1}^{L} |k\rangle = \sum_{ij} K_{j_1 i_2} K_{j_2 i_3} ... K_{j_{L-1} i_L} K_{j_L i_1} |i\rangle_A |j\rangle_B \tag{1.8}$$

The Ansatz satisfies an area-law behaviour, since for any bipartition one cuts two bonds, and thus $S(\rho_L) = 2 \log \chi$ Now we to go back to the original space we can at a time map auxillary states A_s and B_s at a given site s to states of site s using

$$M^s |\psi_{Aux}\rangle = \sum_{i=1}^{d} \sum_{\alpha\beta}^{\chi} A_{\alpha\beta}^{[s]i} |i\rangle \langle\alpha\beta| |\psi_{Aux}\rangle = \sum_{i=1}^{d} Tr[A^{[s]i}] |i\rangle \tag{1.9}$$

Generalizing this to all sites over a chain of lenght L gives us the matrix product state

$$|\psi\rangle_{MPS} = M^1 M^2 ... M^L |\psi_{Aux}\rangle = \sum_{i=1}^{d} \sum_{\{\alpha\}} A_{\alpha_1}^{[1]i_1} A_{\alpha_1\alpha_2}^{[2]i_2} ... A_{\alpha_L}^{[L]i_L} |i_1 i_2 ... i_L\rangle \tag{1.10}$$

where $\{\alpha\} = \{\alpha_1 ... \alpha_{L-1}\}$. The last term is equivalent to taking a trace of the matrix product of A matrices, so

$$|\psi\rangle_{MPS} = \sum_{i=1}^{d} Tr[A^{[1]i_1} A^{[2]i_2} ... A^{[L]i_L}] |i_1 i_2 ... i_L\rangle \tag{1.11}$$

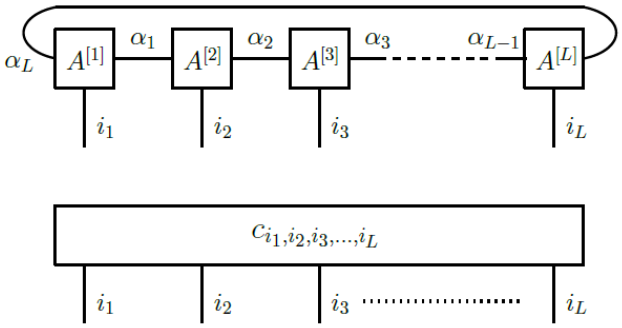

Fig. 1.2: Graphical representation of MPS

Each block is a tensor of rank 3, hence 3 legs. Each vertical leg i corresponds to a site L. The horizontal legs indicate the action of each block on its adjacent block.

1.3 Variational Methods to find the ground state

Now that we can define an MPS for a given system, we use variational optimization protocols to find the ground state of that system. But one must keep in mind that this is useful only in the context of low-dimensional lattice states with local correlations.
Let the local Hamiltonian (for nearest neighbours) be of the form

$$H = \sum_i g(i, i+1) \tag{1.12}$$

where $g(i, i+1)$ is a Hermitian operator that acts both sites i and i+1.

To find the ground state we use the following protocol

1. Let H be your Hammiltonian and $|\psi\rangle_{MPS}$ be the wavefunction defined in (9).
2. Since $|\psi\rangle_{MPS} = |\psi(A^{[2]i_2}...A^{[L]i_L})\rangle$, pick one site s and minimize the functional

$$E = \frac{\langle\psi| H |\psi\rangle}{\langle\psi| |\psi\rangle} \tag{1.13}$$

   as a function of $d\chi^2$ entries of $A^{[s]i}_{\alpha_{s-1}\alpha_s}$
3. Iterate over all lattice sites until energy convergence has been reached.

A point to be noted is that this optimization technique we have presented is rather simplistic and designed for matrix product state. For our results the optimization alogrithm used is far more complicated and beyond the scope of this report.

1.4 A general note on Tensor Network

MPS is the simplest example of a tensor network. There are many kinds of tensor networks for different purposes such as Density Matrix Renormalization Group (both finite and infinite). For our purposes we shall use the heirarchical tensor network MERA.

Chapter 2

Multi-Scale Entanglement Renormalization Ansatz

For quantum systems defined on a lattice, Wilson's RG was used as a prescription to implement Rescaling transformations DMRG is extensively used for 1D systems. Algorithms have been devised to simulate time evolution of 1D and 2D systems.
But they all fail to satisfy the natural requirement of scale invariance at a fixed point [2]. The Hilbert space dimension increases with each rescaling transformation and so does the cost of computation.
Therefore entanglement renormalization was introduced so as to eliminate the growth of the site's Hilbert space dimension along successive rescaling transformations When applied to a scale invariant system the transformation is expected to produce a coarse-grained system identical to the original one.

2.0.1 Isometries

The original Hilbert space was

$$V_L = \otimes_{s=1}^{L} V_s \tag{2.1}$$

For a block B (where a number of sites are grouped),

$$V_B = \otimes_{s \in B} V_s \tag{2.2}$$

After course graining the space $V'_{s'}$ for a site s' $\in$ L' is a subspace of V_B. This mapping is characterized by an isometric tensor w

$$w : V'_{s'} \to V_B \tag{2.3}$$

such that $w^\dagger w = \mathrm{I}$. So basically isometry w maps a state $|\psi\rangle \in V_L$ to a course grained state $|\psi'\rangle \in V_{L'}$

2.0.2 Disentanglers

Selection of the subspace S_B is essential because

1. Its dimension m should be small as computational cost grows polynomially with m.
2. But it should be large enough that $|\psi'\rangle$ should retain the properties of $|\psi'\rangle$.

To do so we need to minimize the entanglement between block B and rest of the lattice L-B. (White) For this we introduce unitary transformations called **disentanglers** which reduces the short range entanglement between block B and its immediate neighbbours.
Let Block be made of two sites s_1 and s_2 with immediate neighbours r to the right and l to the left. Then disentanglers u_1 and u_2 act on the pairs ls_1 and s_2r to reduce the entanglement before them.

$$u_1 : V_l \otimes V_{s_1} \to V_l \otimes V_{s_1} \tag{2.4}$$

and

$$u_2 : V_{s_2} \otimes V_r \to V_{s_2} \otimes V_r \tag{2.5}$$

Remember that these are unitary matrices

$$u_1^\dagger u_1 = I u_2^\dagger u_2 = I \tag{2.6}$$

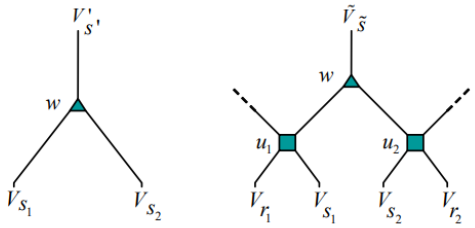

Fig. 2.1: isometries and distentanglers

The above steps lead to course grained lattice with less entanglement. Any observable O can be calculate the from the coarse grained state state $|\tilde{\psi}\rangle$, u, w, 0. This ansatz can be defined for a D dimensional lattice: The Multi-Scale Entanglement Renormalization Ansatz (MERA) consisting of a network of isometric tensors and disentanglers. Our RG transformation is now a 2 step process

1. Use disentanglers to renormalize the entropy between Block B and rest of the system.
2. Use isometries to move to rescaled coarse-grained lattice L′ using support of the density matrix $\tilde{\rho_B}$ of the partially disentangled block B.

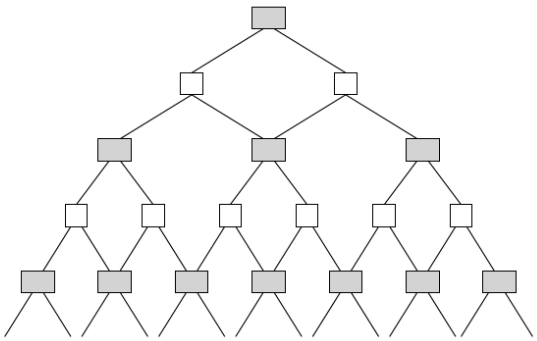

Fig. 2.2: Schematic View of MERA. Grey are disentanglers and white are isometries

Chapter 3

Results

We present our results for the Ising Model. The Hamiltonian for the Ising Model

$$H = -J \sum_{ij} S_i^X S_j^X - h \sum_i S_i^Z \tag{3.1}$$

With periodic boundary conditions, the schematic view of the MERA can be drawn as

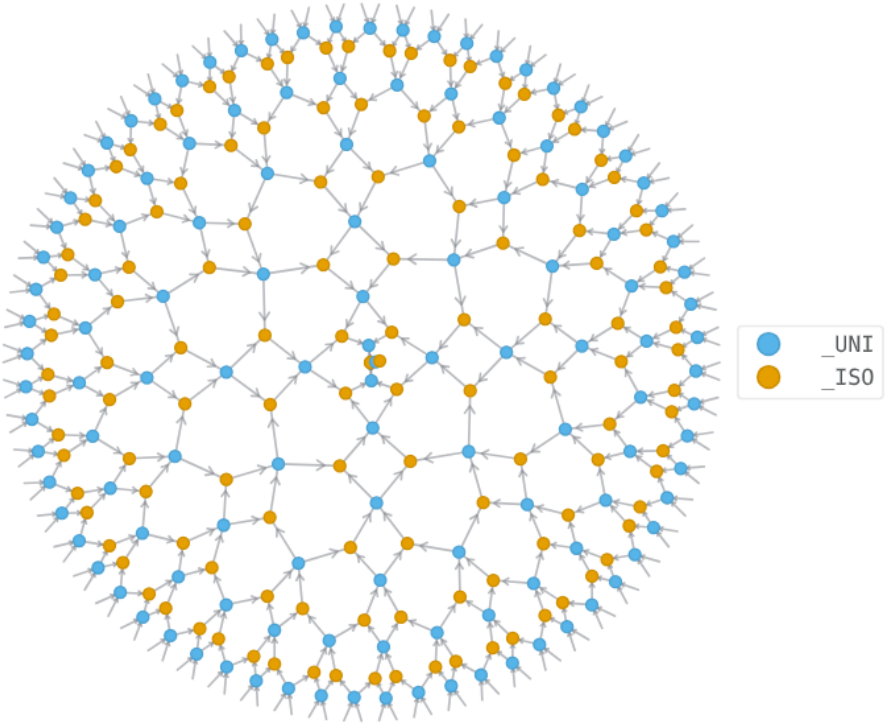

Fig. 3.1: The isometries are orange and unitaries are blue

This figure appears to be circular because the last site is connected to the 1st site. So the outermost layer is rescaled to coarse-grained layers and by doing so one moves inside the circular. The topmost layer in the heirarchy of networks is at the center of the circle.

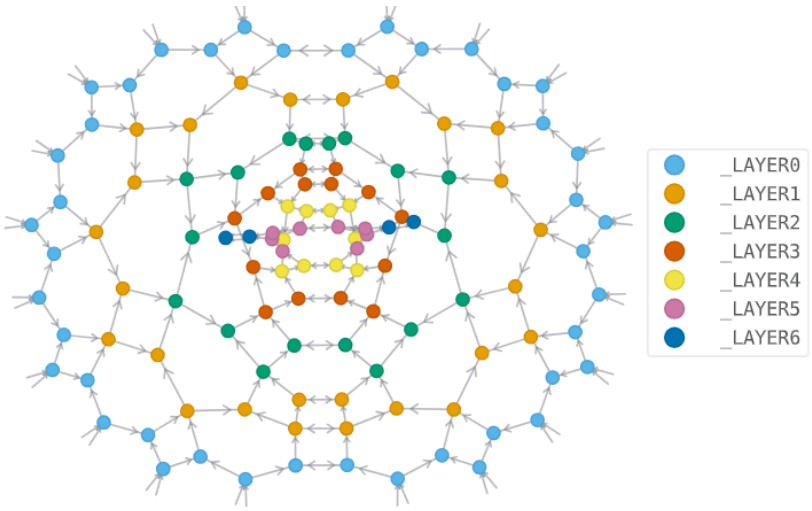

Fig. 3.2: Schematic view of different layers represented by different colors.

3.1 Numerical Results

Using quimb.tensor in python we did the simulation for Ising model with n= 16 sites, J = 1, h=0, i.e. in zero external field.

- Ground state energy pre-optimization = -8.503
- Ground state energy post-optimization = -7.1386

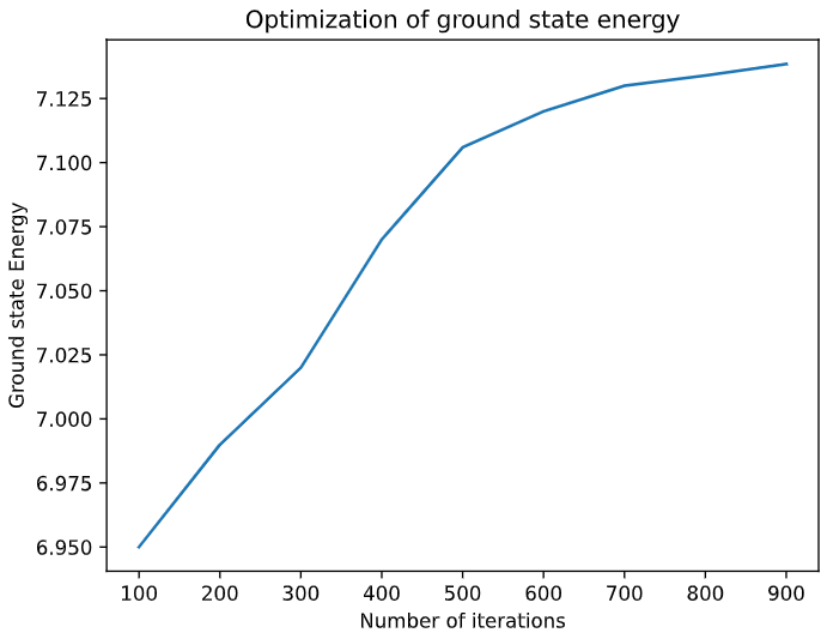

Fig. 3.3: Plot showing the optimiztion of the ground state every 100 iterations

The reason we start with the 100 iterations is that the algorithm quickly reaches a value close to the ground state energy within the first few iterations. After then it slowly evolves to correct the energy to reach a value close to the one obtained before optimization.
Similarly for n= 128 sites, J = 1, h=0

- Ground state energy pre-optimization = -28.374
- Ground state energy post-optimization = -28.16
- Entanglement entropy calculated with partition of 20 sites from the rest of the system

$$\rho = 5.4547 \tag{3.2}$$

- Entanglement entropy between two blocks each of 10 sites

$$\rho = 1.60 \tag{3.3}$$

3.2 Summary and Future Plans

Thus we have calculated the ground state energy for n=16 and n=128 site spin chain in 1D, both before and after optimization with MERA. For the n=16 case we show the variational plot of change in ground state energy until convergence is reached. For n=128 case we also calculate the entanglement entropy between a 20 site block and the rest of the system as well the entropy between two 10 site blocks.
My future plans include the following

- Study of phase transitions
- Maybe... Holographic duality

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