Tensor Network Theory

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What is a tensor ?

A tensor is defined as a series of numbers labeled by N indexes, N called the order of the tensor.

A scalar, which is one number and labeled by zero index, is a 0th-order tensor.

Graphically, we use a dot to represent a scalar

What is a tensor ?

A tensor is defined as a series of numbers labeled by N indexes, N called the order of the tensor.

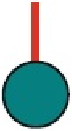
A D-component vector consists of D numbers labeled by one index (first-order tensor).

One can write

$$|\psi\rangle = C_0|0\rangle + C_1|1\rangle = \sum_{s=0,1} C_s|s\rangle,$$

with C are two-component vector.

Graphically, we use a dot with one open bond to represent a vector



What is a tensor ?

A tensor is defined as a series of numbers labeled by N indexes, N called the order of the tensor.

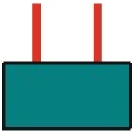
A matrix is in fact a 2nd-order tensor.

The state vector can be written as

$$|\psi\rangle = C_{00}|0\rangle|0\rangle + C_{01}|0\rangle|1\rangle + C_{10}|1\rangle|0\rangle + C_{11}|1\rangle|1\rangle = \sum_{ss'=0}^{1} C_{ss'}|s\rangle|s'\rangle,$$

where $C_{ss'}$ is a matrix with two indexes.

Graphically, we use a dot with two bonds to represent a matrix



Generalities on tensors

What is a tensor ?

A tensor is defined as a series of numbers labeled by N indexes, N called the order of the tensor.

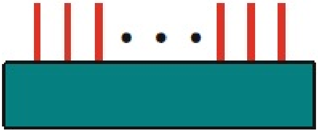
An N-th order tensor.

Considering, N spins, the 2^N coefficients can be written as a N-th order tensor C, satisfying

$$|\psi\rangle = \sum_{s_1 \ldots s'_N = 0}^{1} C_{s_1 \ldots s'_N} |s_1\rangle \ldots |s'_N\rangle.$$

A tensor can be reshaped into a 2^N-component vector.

Graphically, an N-th order tensor is represented by a dot connected with N open bonds



Spin-$1/2$ $\longrightarrow$ each index can take two values.
Spin-S $\longrightarrow$ each index can take $d = 2S + 1$ values,
with d called the bond dimension.
$\widehat{S}^{\alpha}$ $(\alpha = x, y, z)$ is a (2×2) matrix by fixing the basis, where we have

$$S^{\alpha}_{s_1^{'} s_2^{'} s_1 s_2} = < s_1^{'} s_2^{'} | \widehat{S}^{\alpha} | s_1 s_2 > .$$

An N-spin operator can be written as a $2N$-th order tensor.

For instance, we consider to study the quantum entanglement properties, which can be defined by the Schmidt decomposition of the state

$$|\psi> = \sum_{ss'}^{1} |s>|s'> = \sum_{ss'=0}^{1} \sum_{\alpha=0}^{\chi} U_{s\alpha} \lambda_{\alpha\alpha'} V^{*}_{\alpha s'} |s>|s'>,$$

where U and V are unitary matrices,
λ is a positive-defined diagonal matrix in descending order,
χ is called the Schmidt rank.
Note that λ will call the Schmidt coefficient since in the new basis after the decomposition,
the state is

$$|\psi> = \sum_{\alpha} \lambda_{\alpha} |u>_{\alpha} |v>_{\alpha},$$

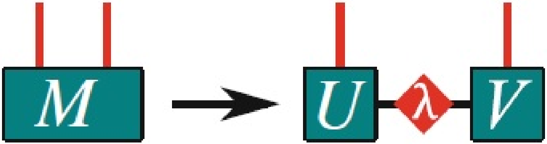
Tensor network and tensor network states

$$|\psi> = \sum_{\alpha} \lambda_\alpha |u>_\alpha |v>_\alpha, (*)$$

with the new basis

$$|u>_\alpha = \sum_s U_{s\alpha}|s> \quad \text{and} \quad |v>_\alpha = \sum_{s'} V^*_{s\alpha}|s'> .$$

Graphically, we have a small tensor network



There are two bonds in the graph shared by two objects, standing for the summations of the two indexes in $(*)$, α and α'.

Matrix Product State (MPS)

Take a N-spin state as an example.
Schollwöck provides a straightforward way to obtain such a tensor network is by repetitively using SVD or QR decomposition.

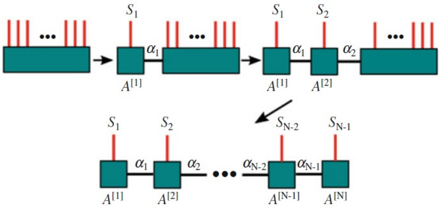


Figure: An impractical way to obtain an MPS from a many-body wave-function is to repetitively use the SVD.

1. Group the first $N-1$ indexes together as one large index,
2. write the coefficients as a $2^{N-1} \times 2$ matrix,
3. implement SVD as the contraction of $C^{[N-1]}$ and $A[N]$.

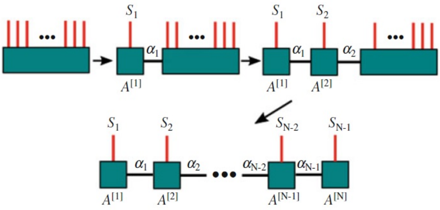


Figure: An impractical way to obtain an MPS from a many-body wave-function is to repetitively use the SVD.

We have

$$C_{s_1 \ldots s_{N-1} s_N} = \sum_{\alpha_{N-1}} C^{[N-1]}_{s_1 \ldots s_{N-1}; \alpha_{N-1}} A^{[N]}_{s_N; \alpha_{N-1}}.$$

For $C[N-1]$, grouping the first $N-2$ indexes

$$C_{s_1 \ldots s_{N-1} \alpha_{N-1}} = \sum_{\alpha_{N-2}} C^{[N-2]}_{s_1 \ldots s_{N-2}; \alpha_{N-2}} A^{[N-1]}_{s_N; \alpha_{N-2} \alpha_{N-1}}.$$

Matrix Product State (MPS)

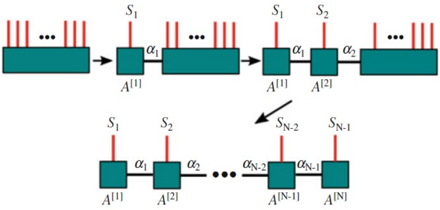


Figure: An impractical way to obtain an MPS from a many-body wave-function is to repetitively use the SVD.

The total coefficients become as

$$C_{s_1 \dots s_{N-1} s_N} = \sum_{\alpha_{N-2}\alpha_{N-1}} C^{[N-2]}_{s_1 \dots s_{N-2};\alpha_{N-2}} A^{[N-1]}_{s_{N-1};\alpha_{N-2}\alpha_{N-1}} A^{[N]}_{s_N;\alpha_{N-1}}.$$

We have the MPS representation of the state as

$$C_{s_1 \dots s_{N-1} s_N} = \sum_{\alpha_1 \dots \alpha_{N-1}} A^{[1]}_{s_1 \dots, \alpha_1} A^{[2]}_{s_2 \dots; \alpha_1 \alpha_2} \dots A^{[N-1]}_{s_{N-1}, \alpha_{N-2}\alpha_{N-1}} A^{[N]}_{s_N, \alpha_{N-1}}.$$

Matrix Product State (MPS)

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One can see that an MPS is a tensor network formed by the contraction of N tensors.
Graphically,

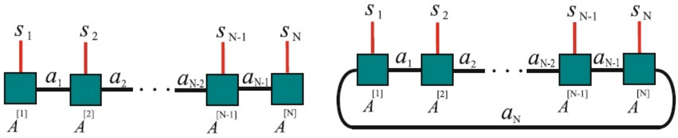

Figure: The graphic representations of the matrix product states with open (left) and periodic (right) boundary conditions.

Matrix Product State (MPS)

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An MPS given in $(**)$ has open boundary condition, and can be generalized to periodic boundary condition as

$$C_{s_1 \ldots s_{N-1} s_N} = \sum_{\alpha_1 \ldots \alpha_{N-1}} A^{[1]}_{s_1 \ldots, \alpha_N \alpha_1} A^{[2]}_{s_2 \ldots; \alpha_1 \alpha_2} \ldots A^{[N-1]}_{s_{N-1}, \alpha_{N-2} \alpha_{N-1}} A^{[N]}_{s_N, \alpha_{N-1} \alpha_N},$$

Where all tensors are third-order.

Afflect-Kennedy-Lieb-Tasaki state

One important example can be found with AKLT model proposed in 1987, a generalization of spin-1 Heisenberg model. For $1D$ systems, Mermin-Wagner theorem forbids any spontaneously breaking of continuous symmetries at finite temperature with sufficiently short-range interactions. For the ground state of AKLT model called AKLT state, it possesses the sparse anti-ferromagnetic order, which provides a non-zero excitation gap under the framework of Mermin-Wagner theorem. Moreover, AKTL state provides us a precious exactly-solvable example to understand edge states and (symmetry-protected) topological orders.

Afflect-Kennedy-Lieb-Tasaki state

Let us begin with the AKLT Hamiltonian that can be given by spin-1 operators as

$$\widehat{H} = \sum_n \left[\frac{1}{2} \widehat{S}_n . \widehat{S}_{n+1} + \frac{1}{6} \left(\left(\widehat{S}_n . \widehat{S}_{n+1} \right)^2 + \frac{1}{3} \right) \right].$$

Non-negative-defined projector $\widehat{P}_2 \left(\widehat{S}_n + \widehat{S}_{n+1} \right)$ that projects the neighboring spins to the subspace of $S = 2$, can be rewritten as

$$\widehat{H} = \sum_n \left(\widehat{S}_n + \widehat{S}_{n+1} \right).$$

Afflect-Kennedy-Lieb-Tasaki state

We put on each site a projector that maps two spins-1/2 to a triplet, the physical spin-1, where the transformation of the basis obeys

$$
\begin{aligned}
|+> &= |00> \\
|\tilde{0}> &= \frac{1}{\sqrt{2}}(|01> + |10>), \\
|-> &= |00> .
\end{aligned}
$$

The corresponding projector is determined by the Clebsch-Gordan coefficients, and is a (3×4) matrix. Here, we rewrite it as a $(3 \times 2 \times 2)$ tensor, whose three components (regarding to the first index) are the ascending, z-component and descending Pauli matrices of spin-1/2,

$$\sigma^{+} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \sigma^{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \sigma^{-} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

We have the tensor A satisfying

$$A_{0,\alpha\alpha'} = \sigma^{+}_{\alpha\alpha'}, \quad A_{1,\alpha\alpha'} = \sigma^{z}_{\alpha\alpha'}, \quad A_{2,\alpha\alpha'} = \sigma^{-}_{\alpha\alpha'}.$$

Then,

$$|\tilde{0}>= \frac{1}{\sqrt{2}}(|01> -|10>).$$

The projector is in fact a (2×2) identity

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

For such an MPS, every projector operator $\widehat{P}_2\left(\widehat{S}_n + \widehat{S}_{n+1}\right)$ in the AKLT Hamiltonian is always acted on a singlet, then we have $\widehat{H}|\psi_{AKLT} >= 0$.

Tree tensor network state (TTNS) and projected entangled pair state (PEPS)

TTNS is a generalization of the MPS that can code more general entanglement states. Unlike an MPS where the tensors are aligned in a $1D$ array, a TTNS is given by a tree graph.

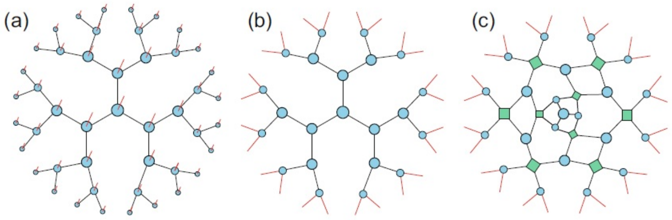

Figure: The illustration of (a) and (b) two different TTNS's and (c) MERA.

Tree tensor network state (TTNS) and projected entangled pair state (PEPS)

An important generalization to the tensor network's of loopy structures is known as projected entangled pair state (PEPS), proposed by Verstraete and Cirac.

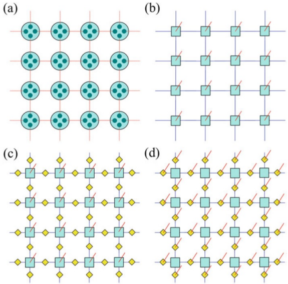

Figure: (a) An intuitive picture of the projected entangled pair state. The physical spins (big circles) are projected to the virtual ones (small circles), which form the maximally entangled states (red bonds). (b)-(d) Three kinds of frequently used PEPS's.

Opens up for further problems

How make contact with MERA being a kind of tensor network states explored in the study of black holes ?

Thank you