TENSOR NETWORKS FOR QUANTUM MANY-BODY SYSTEMS

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In this tutorial...

introducing Tensor Network
States

basic numerical techniques (for QMB systems)
In this session...

Tensor networks? What? Why?

MPS, MPO

PEPS

others
What are tensor networks?
WHAT ARE TNS?

- TNS = Tensor Network States

Context: quantum many body systems

\[ \{ |i\rangle \}_{i=0}^{d-1} \]

interacting with each other

Goal: describe equilibrium states

ground, thermal states
WHAT ARE TNS?

• TNS = Tensor Network States

Context: quantum many body systems

\[ \{ |i\rangle \}_{i=0}^{d-1} \]

interacting with each other

Goal: describe interesting states
ground, thermal states
pictorial representation
tensor = multidimensional array

\{ T_{i_1i_2,j_1j_2,k_1k_2k_3,p} \} \{ i,j,k,p \}
pictorial representation

vector

\[ v_i \quad i = 1, \ldots, D \]

matrix

\[ M_{ij} \quad i = 1, \ldots, D_1 \quad j = 1, \ldots, D_2 \]

a special case

\[ \delta_{ij} \]

\[ i \rightarrow j \rightarrow k \]
contractions

vector

\[ v_i \quad i = 1, \ldots, D \]

\[ u_j \quad j = 1, \ldots, D \]

vector-vector

\[ v \cdot u = \sum_i v_i u_i \]
contractions

matrix

$$M_{ij} \quad i = 1, \ldots, D_1$$

$$u_j \quad j = 1, \ldots, D_2$$

vector

matrix-vector

$$v = M \cdot u = \sum_j M_{ij} u_j$$
computational costs

v \cdot u = \sum_i v_i u_i

v = M \cdot u = \sum_j M_{ij} u_j

M \cdot N = \sum_j M_{ij} N_{jk}

in general: product of open and contracted dimensions
basic routines

\[ M = U S V^\dagger \]

\[ O(Dd^2) \]
basic routines

SVD

\[ M = U S V^\dagger \]

\[ \text{trace} \]

\[ \sum_{ij} M_{ij} \delta_{ij} = \sum_{i} M_{ii} = \text{tr} M \]

\[ \text{partial trace} \]

\[ \sum_{ij} M_{ia,jb} \delta_{ij} = \sum_{i} M_{ia,ib} = \text{tr}_d M \]
pictorial representation
WHAT ARE TNS?

- TNS = Tensor Network States

A general state of the N-body Hilbert space has exponentially many coefficients:

$$|\Psi\rangle = \sum_{i_j} c_{i_1...i_N} |i_1...i_N\rangle$$

A TNS has only a polynomial number of parameters:

poly($N$)

$\mathcal{d}^N$
WHAT ARE TNS?

- TNS = Tensor Network States

A particular example

Mean field approximation

product state

Can still produce good results in some cases
WHY SHOULD TNS BE USEFUL?

States appearing in Nature are peculiar

State at random from Hilbert space is not close to product

\[ H \]

\text{product states}

• TNS = Tensor Network States
WHY SHOULD TNS BE USEFUL?

States appearing in Nature are peculiar

State at random from Hilbert space is not close to product

We look for the particular "corner" of the Hilbert space

- TNS = Tensor Network States
WHY SHOULD TNS BE USEFUL?

The goal is to find good descriptions of physical states

WANTED

⇒ efficient representation
⇒ computable observables
⇒ (variational) algorithms
FINDING A GOOD ANSATZ

Which properties characterize physically interesting states?

ENTANGLEMENT STRUCTURE

\[ |a\rangle \otimes |b\rangle + |b\rangle \otimes |a\rangle \]

\[ S(A) = -\text{tr}(\rho_A \log(\rho_A)) \]

entanglement entropy
FINDING A GOOD ANSATZ

Which properties characterize ground states of relevant Hamiltonians?

- finite range
- gapped
- states with little entanglement

Area law
FINDING A GOOD ANSATZ

Which properties characterize ground states of relevant Hamiltonians?

Local gapped 1D Hamiltonians have ground states with area law of entanglement

\[ S_{A_{\text{max}}} \propto |\delta A| \quad \text{Hastings 2007} \]

in 1D critical systems, logarithmic corrections

\[ S_{A_{\text{max}}} \propto |\delta A| \log A \quad \text{Calabrese, Cardy 2004} \]

satisfied at finite temperature \hspace{1cm} \text{Wolf, Verstraete, Hastings, Cirac, PRL 2008}
MPS & PEPS

• MPS = Matrix Product States

• PEPS = Projected Entangled Pairs States

Ansätze satisfying the area law by construction

TNS = entanglement based ansatz
**TNS = entanglement based ansatz**

Area law

**other TNS**

TTN

Suggested connection to AdS/CFT

MERA

Vidal PRL 2007

Swingle PRD 2012

Molina JHEP 2013

Nozaki et al JHEP 2012

Bao et al PRD 2015


MPS
MPS
Matrix Product States
A bit of history...

AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

\[ H_{ii+1} = \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \]

The ground state is exactly a MPS (VBS)

\( S = \frac{1}{2} \)
AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

\[ H_{ii+1} = \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \]

The ground state is exactly a MPS (VBS)
MPS
Matrix Product States

A bit of history...

AKLT exactly solvable spin model
Affleck, Kennedy, Lieb, Tasaki, PRL 1987

Finitely correlated states
Fannes, Nachtergaele, Werner, CMP 1992

DMRG algorithm
White, PRL 1992

DMRG variational over MPS
Ostlund, Rommer, PRL 1995

Quantum Information perspective
Vidal, PRL 2003
Verstraete, Porras, Cirac, PRL 2004
Matrix Product States (MPS)

|\psi\rangle = \sum_{i_1 \ldots i_N} \text{tr}(A_{i_1}^{i_1} A_{i_2}^{i_2} \ldots A_{i_N}^{i_N}) |i_1 \ldots i_N\rangle

Area law by construction

Bounded entanglement \( S(L/2) \leq \log D \)

Number of parameters \( N d D^2 \)
MPS EXAMPLE

\[ |\Psi\rangle = \sum_{i_1 \ldots i_N} \text{tr}(A_{i_1}^1 A_{i_2}^2 \ldots A_{i_N}^N)|i_1 \ldots i_N\rangle \]

\[
A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad A^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}
\]

\[ |100 \ldots\rangle + |010 \ldots\rangle + |001 \ldots\rangle + \ldots \]

\[ D = 2 \]
MPS
Matrix Product States

maximally entangled
\[ \sum_{\alpha=1}^{D} |\alpha\rangle|\alpha\rangle \]

physical site

virtual particles

virtual particles
maximally entangled
\[ \sum_{\alpha=1}^{D} |\alpha\rangle|\alpha\rangle \]

project onto the physical degrees of freedom
\[ \sum_{i\alpha\beta} A^i_{\alpha\beta} |i\rangle\langle\alpha\beta| \]

virtual particles

Area law by construction

Bounded entanglement

\[ S(L/2) \leq \log D \]
MPS PROPERTIES

Area law by construction
MPS PROPERTIES

Area law by construction

\[ S(\bullet \bullet) \leq S(\ldots\ldots) \]

\[ = S(\ldots) \]

\[ = 2\log D \]

Local projectors cannot increase the entropy.
SOME OTHER PROPERTIES
MPS PROPERTIES

any state can be written as MPS

\[ D \leq d^{N/2} \]
MPS PROPERTIES

MPS are a complete family increasing the bond dimension, they can describe any state of the Hilbert space

\[ D \leq d^{N/2} \]

- \( D = 1 \)
- \( D = 2 \)
- \( D = 3 \)
MPS PROPERTIES

\[ X \cdot X^{-1} \]

gauge freedom

Pérez-García, Verstraete, Wolf, Cirac, Q.Inf.Comp. 2007
MPS PROPERTIES

canonical form

$$\sum_i A^{[m]i} A^{[m]i\dagger} = 1$$

$$\sum_i A^{[m]i\dagger} \Lambda^{[m-1]} A^{[m]i} = \Lambda^{[m]}$$

unique
imposed locally

gauge freedom
MPS PROPERTIES

finding the canonical form

\[ D D D = \text{SVD} \]
MPS PROPERTIES

finding the canonical form
MPS PROPERTIES

finding the canonical form
MPS PROPERTIES

Efficient expectation values

\[ |\Psi\rangle = \sum_{\{i_k\}} c_{i_1i_2...i_N} |i_1i_2...i_N\rangle \]
MPS PROPERTIES

Efficient expectation values

\[\langle \Psi | O | \Psi \rangle = \sum_{\{i_k, j_k\}} c_{i_1i_2...i_N}^* c_{j_1j_2...j_N} \langle i_1i_2...i_N | O | j_1j_2...j_N \rangle\]
**MPS PROPERTIES**

Efficient expectation values

\[ \langle \Psi | O^{[M]} | \Psi \rangle = \sum_{\{i_k\}_{k \neq M}} \sum_{i_M,j_M} c^*_1 \ldots c^*_M \ldots c^*_N c_1 \ldots c_M \ldots c_N \langle i_1 | O | j_M \rangle \]
MPS PROPERTIES

Efficient expectation values

\[ E = \sum_i A^i \otimes A^i \]
MPS PROPERTIES

Efficient expectation values

\[ E_O = \sum_{ij} A^i \otimes A^j \langle i | O | j \rangle \]

transfer operator

\( D^2 \times D^2 \) matrix
MPS PROPERTIES

Efficient expectation values

$O(D^4)$
MPS PROPERTIES

Exponentially decaying correlations

\[ \langle A^p B^{p+x} \rangle - \langle A^p \rangle \langle B^{p+x} \rangle \]
MPS PROPERTIES

Exponentially decaying correlations

\[ \langle A[p] B[p+x] \rangle \]

\[ \lambda_1^{x-1} \left( |R_1 \rangle \langle L_1| + \left( \frac{\lambda_2}{\lambda_1} \right)^{x-1} |R_2 \rangle \langle L_2| + \ldots \right) \]

\[ E = \sum_i A^i* \otimes A^i = \sum_k \lambda_k |R_k \rangle \langle L_k| \]
MPS PROPERTIES

Exponentially decaying correlations

\[ \langle A^{[p]} B^{[p+x]} \rangle \]

\[ \lambda_1^{x-1} \left( |R_1\rangle \langle L_1| + \left( \frac{\lambda_2}{\lambda_1} \right)^{x-1} |R_2\rangle \langle L_2| + \ldots \right) \]

normalize

disconnected component

exponential decrease
MPS PROPERTIES

Efficient preparation

equivalent to an ancilla with dimension \( D \)
MPS PROPERTIES

Approximate ground states efficiently

\[ |\Psi\rangle \approx |\Psi_D\rangle \]

\[ \| |\Psi\rangle - |\Psi_D\rangle \|^2 \leq 2 \sum_{\alpha=1}^{N-1} \epsilon_\alpha(D) \]

\[ \epsilon_\alpha(D) = \sum_{k=D+1}^{M_\alpha} \mu_k^{(\alpha)} \]

\text{truncation per link}

\text{squared Schmidt values}

\text{quality of approximation depends on how fast Schmidt values decay}

\text{for ground states of local gapped 1D Hamiltonians}

\[ \epsilon_\alpha(D) \leq CD^{-\frac{1}{\xi' \log d}} \]

Hastings JStatMech 2007
MPS PROPERTIES

Also periodic boundary conditions

more expensive (still efficient) contractions $O(D^5)$

could be written as OBC with $D^2$

(twice the entropy at half chain)
MPS PROPERTIES

local parent Hamiltonian

Generalization of AKLT construction

\[
S_2
\]

\[
X \in \mathbb{C}^{D \times D}
\]

\[
H = \sum_{i=1}^{N-1} (1 - \Pi_{S_2})
\]

local, frustration-free

MPS injectivity \iff unique ground state
MPS PROPERTIES

Symmetries

fundamental physical concept

invariant Hamiltonian $\rightarrow$ symmetric (covariant) eigenstate

$$ UHU^\dagger = H \quad U|E_n\rangle = e^{i\phi}|E_n\rangle $$

restrict effective Hilbert space to given quantum numbers

role of tensors symmetry?
MPS PROPERTIES

Tensors can be symmetric $\Rightarrow$ state invariant

Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010
MPS PROPERTIES

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state invariant $\Leftrightarrow$

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MPS PROPERTIES

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Tensors can be symmetric $\Rightarrow$ state invariant

For MPS and PEPS, there is a canonical form

\[ U_g \]

state invariant $\Leftrightarrow$

In general: structure of tensor $\Rightarrow$
symmetry properties

gauge symmetries
Tagliacozzo et al. PRX 2014
Haegeman et al. PRX 2015

topological order
Wahl et al., PRL 2013
Sahinoglu et al. arXiv:1409.2150
MPS PROPERTIES

RECAP

good approximation of ground states
  gapped finite range Hamiltonian \rightarrow
  area law (ground state)

efficient calculation of expectation values
  exponentially decaying correlations

can be prepared efficiently
PEPS
Projected Entangled Pairs

natural generalization of MPS
PEPS
Projected Entangled Pairs States

area law by construction

any lattice

local map onto the physical d.o.f.

additional virtual particles
PEPS
Projected Entangled Pairs States

area law by construction

any lattice

Entropy of a region bounded by the number of cut bonds
PEPS
Projected Entangled Pairs States

area law by construction

any lattice

Entropy of a region bounded by the number of cut bonds
PEPS
Projected Entangled Pairs States

$D$: virtual bond

d: physical bond

Computing the norm

$|\Psi\rangle$

$\langle \Psi |$
PEPS
Projected Entangled Pairs States

$D^2 \times D^2$
PEPS
Projected Entangled Pairs States

$D^2$

$D^4 \times D^2$
PEPS
Projected Entangled Pairs States

\[ D^2 \times D^6 \]
PEPS
Projected Entangled Pairs States

$D^2 \times D^2$

contracting #P-complete
Best we can do: approximate (e.g. via MPO-MPS contractions)

PEPS
Projected Entangled Pairs States

Needed for expectation values and tensor updates
PEPS
Projected Entangled Pairs States

local parent Hamiltonian

$$H = \sum_{i=1}^{N-1} (1 - \Pi_{S_2})$$
local, frustration-free injectivity \(\Rightarrow\) unique ground state

bulk-boundary correspondence

holographic principle: boundary dof determine physics in bulk

half-system RDM on virtual dof
map virtual to physical
PEPS
Projected Entangled Pairs States

Properties

no efficient calculation of expectation values

- can hold algebraically decaying correlations

cannot be prepared efficiently

ground state of local frustration-free Hamiltonians

efficient approximation of thermal states

Hastings PRB 2006
Molnar et al PRB 2015