Tensor Networks   Summer semester, 2023   Jan von Delft   TNB-I.0

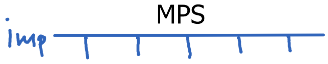
Why study tensor networks? Because tensor networks provide a flexible description of quantum states.
They encode entanglement between subsystems in the bonds linking the tensors of the network.

Course outline:

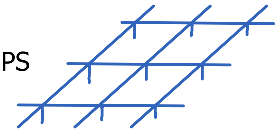
- Tensor network basics
- Matrix product states (MPS): 1d tensor networks
- (Optional: Symmetries - Qspace)
- Density Matrix Renormalization Group (DMRG) for 1d quantum lattices models
- Numerical Renormalization Group (NRG) for quantum impurity models
- Projected Entangled Pair States (PEPS) for 2d quantum lattice models
- Various Tensor Renormalization Group (TRG) approaches
- Machine learning with tensor networks

MPS

MPS



PEPS



References: consult the bibtex file TensorNetworkLiterature.bib on course website → References

Lecture 01: Tensor networks basics I

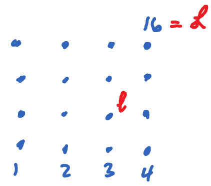
1. Notation for generic quantum lattice system
2. Entanglement and Area Laws
3. Tensor network diagrams (graphical conventions)

1. Notation for generic quantum lattice system

TNB-I.1

For concreteness, we introduce some general notation for describing a generic quantum lattice system.

Think of spin- S lattice in arbitrary dimensions, with $\mathcal{L}$ sites, enumerated by an index $\ell = 1, \dots, \mathcal{L}$



Local state space of site ℓ : $\quad |\sigma_\ell\rangle_\ell \in \{|1\rangle_\ell, |2\rangle_\ell, \dots |2S+1\rangle_\ell\}$ (1)

Local state label: $\quad \sigma_\ell = 1, 2, \dots, 2S+1$ (2)

Local dimension: $\quad d = 2S+1$ (3)

Shorthand: $\quad |\sigma_\ell\rangle := |\sigma_\ell\rangle_\ell$ (4)

Index ℓ on state label σ_ℓ suffices to identify the site Hilbert space $|\ \rangle_\ell$

Generic basis state for full system of $\mathcal{L}$ sites (convention: add state spaces for new sites from the right):

$$|\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \dots \otimes |\sigma_\ell\rangle \otimes \dots |\sigma_\mathcal{L}\rangle := |\sigma_1, \sigma_2, \dots, \sigma_\ell, \dots, \sigma_\mathcal{L}\rangle := |\vec{\sigma}\rangle_\mathcal{L} \quad (5)$$

$\leftarrow$ identifies length of chain

Hilbert space for full chain: $\quad \mathcal{H}^\mathcal{L} = \mathrm{span}\{|\vec{\sigma}_\mathcal{L}\rangle\}$ (6)

General quantum state: $\quad |\psi\rangle_\mathcal{L} = \sum_{\sigma_1, \dots, \sigma_\mathcal{L}} |\sigma_1, \dots, \sigma_\mathcal{L}\rangle C^{\sigma_1, \dots, \sigma_\mathcal{L}} := |\vec{\sigma}\rangle C^{\vec{\sigma}}$ (7)

$(\in \mathcal{H}^\mathcal{L})$

arbitrary linear combinations

wavefunction

summation over repeated indices implied

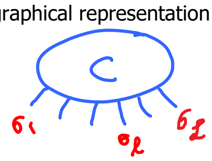
Dimension of full Hilbert space $\mathcal{H}^\mathcal{L}$: $\quad d^\mathcal{L}$ (# of different configurations of $\vec{\sigma}_\mathcal{L}$)

Specifying $|\psi\rangle_\mathcal{L}$ involves specifying $C^{\vec{\sigma}}$, i.e. $d^\mathcal{L}$ different complex numbers.

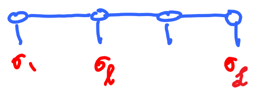
$C^{\vec{\sigma}} = C^{\sigma_1, \dots, \sigma_\mathcal{L}}$ is a tensor of degree $\mathcal{L}$ (8)

number of legs

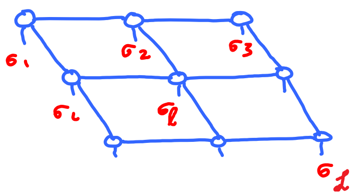
graphical representation



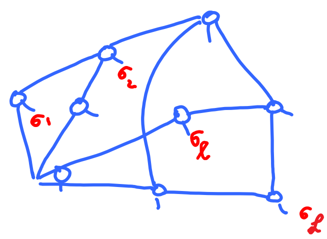
Claim (to be made plausible later): such a degree $\mathcal{L}$ tensor can be represented in many different ways:



MPS: matrix product state



PEPS: projected entangled-pair state



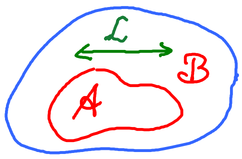
arbitrary tensor network

We will see:

- a link between two sites represents entanglement between them
- different representations $\Rightarrow$ different entanglement book-keeping
- tensor network = entanglement representation of a quantum state

2. EntanglementeEntropy and area laws

Consider quantum system in pure state $|\psi\rangle$, with density matrix $\hat{\rho} = |\psi\rangle\langle\psi|$



Divide system into two parts, $\mathcal{A}$ and $\mathcal{B}$. Suppose $\mathcal{A}$ has linear dimension $\mathcal{L}$.

E.g. $\mathcal{H}_{\mathcal{A}} = \mathrm{span}\{|\vec{\sigma}_{\mathcal{A}}\rangle\}$, $\mathcal{H}_{\mathcal{B}} = \mathrm{span}\{|\vec{\sigma}_{\mathcal{B}}\rangle\}$

number of sites (dimensionless)

To obtain reduced density matrix of $\mathcal{A}$ (or $\mathcal{B}$), trace out $\mathcal{B}$ (or $\mathcal{A}$):

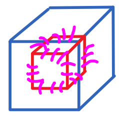
'reduced density matrix' for $\mathcal{A}$: $\hat{\rho}_{\mathcal{A}} := \mathrm{Tr}_{\mathcal{B}}\, \hat{\rho}$ and $\hat{\rho}_{\mathcal{B}} := \mathrm{Tr}_{\mathcal{A}}\, \hat{\rho}$ (1)

'Entanglement entropy' of $\mathcal{A}$ and $\mathcal{B}$: $S_{\mathcal{A}/\mathcal{B}} = -\mathrm{Tr}_{\mathcal{A}}\, \hat{\rho}_{\mathcal{A}} \log_2 \hat{\rho}_{\mathcal{A}} = -\sum_{\alpha} w_{\alpha} \log_2 w_{\alpha}$ (2)

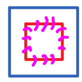
eigenvalues of $\hat{\rho}_{\mathcal{A}}$

Remarkable fact: for Hamiltonians with only local interactions, the ground state entanglement entropy is governed by an 'area law' [Hastings2007,Eisert2010,Cirac2021]:

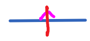
$S := S_{\mathcal{A}/\mathcal{B}} \sim$ (area of boundary of $\mathcal{A}$) $\equiv \partial\mathcal{A}$ (3)



$\sim \mathcal{L}^2$ in 3D for gapped system (3a)



$\sim \mathcal{L}$ in 2D for gapped system (3b)



$\sim$ const. in 1D for gapped system (3c)

$\sim$ const. $+ \ln \mathcal{L}$ in 1D for gapless system (3d)

Area law has consequences for the numerical costs required for adequately encoding the entanglement in tensor network descriptions of the ground state. To see this, we review some basic properties of reduced density matrices.

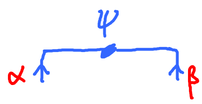
Suppose the two subsystems, $\mathcal{A}$ and $\mathcal{B}$, are defined on Hilbert spaces with

with dimensions D and D', and orthonormal bases $\{|\alpha\rangle_{\mathcal{A}}\}$ and $\{|\beta\rangle_{\mathcal{B}}\}$.

Here α and β enumerate all basis states of Hilbert spaces of $\mathcal{A}$ and $\mathcal{B}$, respectively.

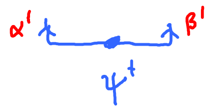
General form of pure state on $\mathcal{A} \cup \mathcal{B}$: graphical notation

$|\psi\rangle = |\alpha\rangle_{\mathcal{A}} |\beta\rangle_{\mathcal{B}}\, \psi^{\alpha\beta}$



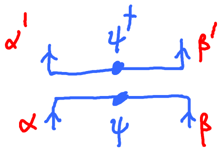
(4a)

$\langle\psi| = \underbrace{\psi^{\dagger}_{\beta'\alpha'}}_{:=\ \psi^{\alpha'\beta'}}\, {}_{\mathcal{B}}\langle\beta'|\, {}_{\mathcal{A}}\langle\alpha'|$



(4b)

Density matrix: $\hat{\rho} = |\psi\rangle\langle\psi|$



(4c)

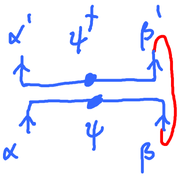
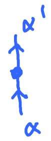
Reduced density matrix of subsystem $\mathcal{A}$:

$$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}} |\psi\rangle\langle\psi| = \sum_{\bar{\beta}} {}_{\mathcal{B}}\langle\bar{\beta}|\alpha\rangle_{\mathcal{A}} |\beta\rangle_{\mathcal{B}} \psi^{\alpha\beta} \psi^{\dagger}_{\beta'\alpha'} {}_{\mathcal{B}}\langle\beta'| {}_{\mathcal{A}}\langle\alpha'|\bar{\beta}\rangle_{\mathcal{B}} \quad (5)$$

$$= |\alpha\rangle_{\mathcal{A}} (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} {}_{\mathcal{A}}\langle\alpha'|$$

with

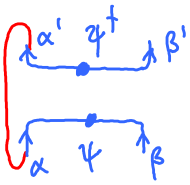
$$(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = \sum_{\bar{\beta}} \underbrace{{}_{\mathcal{B}}\langle\bar{\beta}|\beta\rangle_{\mathcal{B}}}_{\delta^{\bar{\beta}}{}_{\beta}} \psi^{\alpha\beta} \psi^{\dagger}_{\beta'\alpha'} \underbrace{{}_{\mathcal{B}}\langle\beta'|\bar{\beta}\rangle_{\mathcal{B}}}_{\delta^{\beta'}{}_{\bar{\beta}}} = \psi^{\alpha\beta} \underbrace{\psi^{\dagger}_{\beta\alpha'}} \equiv (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'} \quad (6)$$

$(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} =$  $=$  $\psi^{\alpha\beta} \psi^{\dagger}_{\beta\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'}$ (7)

Analogously: reduced density matrix of subsystem $\mathcal{B}$:

$$\hat{\rho}_{\mathcal{B}} = \mathrm{Tr}_{\mathcal{A}} |\psi\rangle\langle\psi| = |\beta\rangle_{\mathcal{B}} (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} {}_{\mathcal{B}}\langle\beta'| \quad \text{with} \quad (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} = (\psi^{\dagger}\psi)_{\beta'}{}^{\beta} \quad (8)$$

Diagrammatic derivation:

$(\rho_{\mathcal{B}})^{\beta}{}_{\beta'} =$  $=$  $\psi^{\alpha\beta} \psi^{\dagger}_{\beta'\alpha} = (\psi^{\dagger}\psi)_{\beta'}{}^{\beta}$ (9)

Algebraic derivation:

$$(\rho_{\mathcal{B}})^{\beta}{}_{\beta'} = \sum_{\bar{\alpha}} \underbrace{{}_{\mathcal{A}}\langle\bar{\alpha}|\alpha\rangle_{\mathcal{A}}}_{\delta^{\bar{\alpha}}{}_{\alpha}} \psi^{\alpha\beta} \psi^{\dagger}_{\beta'\alpha'} \underbrace{{}_{\mathcal{A}}\langle\alpha'|\bar{\alpha}\rangle_{\mathcal{A}}}_{\delta^{\alpha'}{}_{\bar{\alpha}}} = \psi^{\dagger}_{\beta'\alpha} \psi^{\alpha\beta} =: (\psi^{\dagger}\psi)_{\beta'}{}^{\beta} \quad (10)$$

Now it is always possible to find bases for the Hilbert spaces of $\mathcal{A}$ and $\mathcal{B}$ in which both reduced density matrices $\hat{\rho}_{\mathcal{A}}$ and $\hat{\rho}_{\mathcal{B}}$ are diagonal. (Tool to achieve this: 'singular value decomposition', see Sec. TNB-II.1.)

E.g. for $\hat{\rho}_{\mathcal{A}}$: $(\psi\psi^{\dagger})^{\alpha}{}_{\alpha'} = \delta^{\alpha}{}_{\alpha'} w_{\alpha}$ eigenvalues with $\alpha = 1, \dots D$ 'bond dimension' (11)

Normalization $$1 = \mathrm{Tr}\,\hat{\rho}_{\mathcal{A}} = \sum_{\alpha} w_{\alpha} \quad (12)$$

Entanglement entropy: $$S \overset{(2)}{=} -\sum_{\alpha=1}^{D} w_{\alpha} \log_2 w_{\alpha} \quad (13a)$$

Maximal if $w_{\alpha} = \frac{1}{D}$ for all α : $$\leq -\sum_{\alpha=1}^{D} \frac{1}{D} \log_2 \frac{1}{D} = \log_2 D \quad (13b)$$

$$\Rightarrow \quad \boxed{2^{S} \leq D} \quad (14)$$

$$\Rightarrow \quad \boxed{2^{S} \leq D} \tag{14}$$

To fully capture entanglement between subsystems $\mathcal{A}$ and $\mathcal{B}$, the reduced density matrix dimension D must satisfy

1D gapped: $D \overset{(3c)}{\sim} 2^{\text{const}}$ (independent of system size!) (15a)

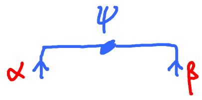
1D critical: $\overset{(3d)}{\sim} 2^{\text{const} + \ln} \sim$ power law in L (15b)

2D gapped: $\overset{(3b)}{\sim} 2^{L}$ (15c)

3D gapped: $\overset{(3a)}{\sim} 2^{L^2}$ (15d)

> Important conclusion: for gapped and gapless systems in 1D,
> ground state entanglement can be encoded efficiently using limited numerical resources.
> For 2D or 3D systems, numerical costs grow exponentially.

In $|\psi\rangle = |\alpha\rangle_{\mathcal{A}} |\beta\rangle_{\mathcal{B}} \, \psi^{\alpha\beta}$



the entanglement between subsystems $\mathcal{A}$ and $\mathcal{B}$ is encoded in the two-index tensor $\psi^{\alpha\beta}$

Quite generally, <u>entanglement</u> between subsystems can be encoded via <u>tensors</u>. For several connected subsystems (e.g. lattice sites), this leads to a description in terms of <u>tensor networks</u>.

3. Tensor network diagrams

[Orus 2014, Sec. 4.1]

TNB-I.3

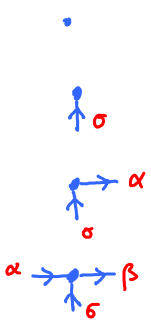
'tensor' = multi-dimensional array of numbers

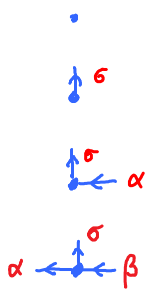
'rank of degree' = number of indices = # of legs

'dimension of leg' = number of values taken by its index, $\alpha = 1, \dots, D_\alpha$

overbar denotes complex conjugation

degree-0:	scalar	A	$A^\dagger := \bar{A}$
degree-1:	vector	A^σ	$A^\dagger{}_\sigma := \overline{A^\sigma}$
degree-2:	matrix	$A^\sigma{}_\alpha$	$A^{\dagger\alpha}{}_\sigma := \overline{A^\sigma{}_\alpha}$
degree-3:	tensor	$A^{\alpha\sigma}{}_\beta$	$A^{\dagger\beta}{}_{\sigma\alpha} := \overline{A^{\alpha\sigma}{}_\beta}$

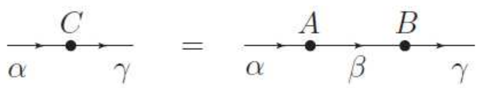




[Our conventions for using arrows and distinguishing between super- and subscripts ('covariant notation') will be explained in Sec. TNB-II.1. In short: incoming = upstairs, outgoing = downstairs. Use of covariant notation is not customary in tensor network litertarure - most authors write all indices downstairs, and you may do so too. However, covariant notation does become useful when exploiting non-Abelian symmetries.]

Index contraction: summation over repeated index

$$C^\alpha{}_\gamma = \sum_{\beta=1}^{D_\beta} A^\alpha{}_\beta B^\beta{}_\gamma \equiv A^\alpha{}_\beta B^\beta{}_\gamma$$



graphical representation of matrix product

D_β = 'bond dimension' of index β

(depends on context, can be different for each index; the subscript β on D_β is often/usually not written explicitly)

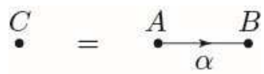
'open index' = non-contracted index (here α , γ)

'tensor network' = set of tensors with some or all indices contracted according to some pattern

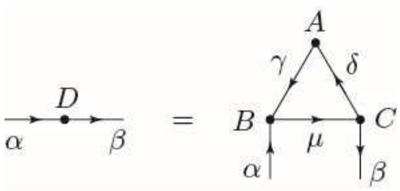
Examples:

$$C = A_\alpha B^\alpha$$

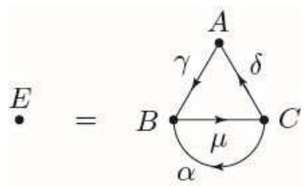
scalar   dual vector · vector



$$D^\alpha{}_\beta = A^\delta{}_\gamma B^{\gamma\alpha}{}_\mu C^\mu{}_{\beta\delta}$$

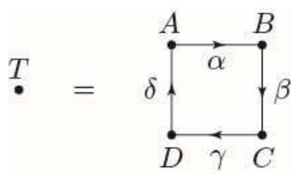


$$E = D^\alpha{}_\alpha = A^\delta{}_\gamma B^{\gamma\alpha}{}_\mu C^\mu{}_{\alpha\delta}$$



Trace of matrix product:

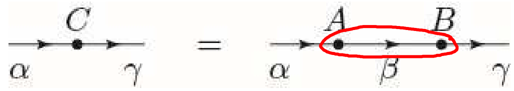
$$T = A^\delta{}_\alpha B^\alpha{}_\beta C^\beta{}_\gamma D^\gamma{}_\delta$$



Cost of computing contractions

Result of contraction does not depend on order in which indices are summed, but numerical cost does !

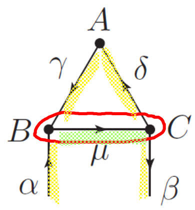
Example 1: cost of matrix multiplication is $\mathcal{O}(D^3)$:



For every fixed α and γ ($D_\alpha \times D_\gamma$ combinations), sum over D_β values of β

Cost = $D_\alpha \cdot D_\gamma \cdot D_\beta$ (simplifies to D^3 if all bond dimensions are = D)

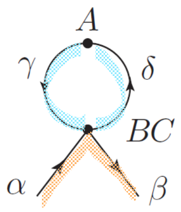
Example 2:



4 legs , 1 sum

$\mathcal{O}(D^4 \cdot D)$

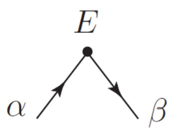
contracting μ



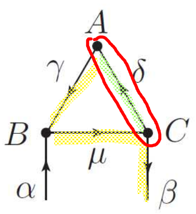
2 legs , 2 sums

$\mathcal{O}(D^2 \cdot D^2)$

contracting $\gamma\delta$



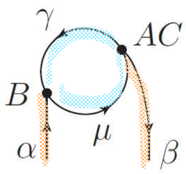
$$A^{\delta}{}_{\gamma}\, B^{\gamma\alpha}{}_{\underbrace{\mu\, C^{\mu}}}{}_{\beta\delta} = \underbrace{A^{\delta}{}_{\gamma}\, (BC)^{\gamma\alpha}{}_{\beta\delta}} = E^{\alpha}{}_{\beta}$$



3 legs , 1 sum

$\mathcal{O}(D^3 \cdot D)$

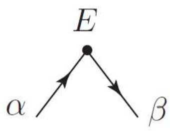
contracting δ



2 legs , 2 sums

$\mathcal{O}(D^2 \cdot D^2)$

contracting $\gamma\mu$



$$B^{\gamma\alpha}{}_{\mu}\, \underbrace{\overline{A^{\delta}{}_{\gamma}\, C^{\mu}{}_{\beta\delta}}}_{\text{independent of } \alpha\ !!} = \underbrace{B^{\gamma\alpha}{}_{\mu}\, (AC)^{\mu}{}_{\beta\gamma}} = E^{\alpha}{}_{\beta}$$

First contraction scheme has total cost $\mathcal{O}(D^5)$, second has $\mathcal{O}(D^4)$!!

Finding optimal contraction order is difficult problem! In practice: rely on experience, trial and error...

Next sections:

- Covariant index notation, arrow conventions
- Iterative diagonalization of a chain
- Singular value decomposition (needed for finding efficient representations of entanglement)
- Schmidt decomposition (most efficient way of representing entanglement)