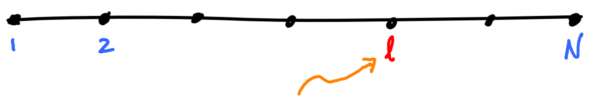
Tensor Network Basics (TNB-I)

TNB-I.1

1. Why study tensor networks? (Intro)

Because tensor networks provide a flexible description of quantum states.

Example: spin- S chain, with N sites



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: $\quad \sigma = 1, 2, \dots, 2S+1$ (2)

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

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

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

Generic basis state for full chain of length N (convention: add state spaces for new sites from the left):

$$|\sigma_N\rangle \otimes \dots \otimes |\sigma_\ell\rangle \otimes \dots |\sigma_2\rangle \otimes |\sigma_1\rangle \equiv |\sigma_1, \sigma_2, \dots, \sigma_\ell, \dots, \sigma_N\rangle = |\vec{\sigma}\rangle_N \tag{5}$$

N identifies length of chain

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

General quantum state: $(\in \mathcal{H}^N)$

$$|\psi\rangle_N = \sum_{\sigma_1, \dots, \sigma_N} |\sigma_1, \dots, \sigma_N\rangle C^{\sigma_1, \dots, \sigma_N} \equiv C^{\vec{\sigma}} |\vec{\sigma}\rangle_N \tag{7}$$

arbitrary linear superpositions

wavefunction

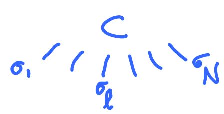
summation over repeated indices implied

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

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

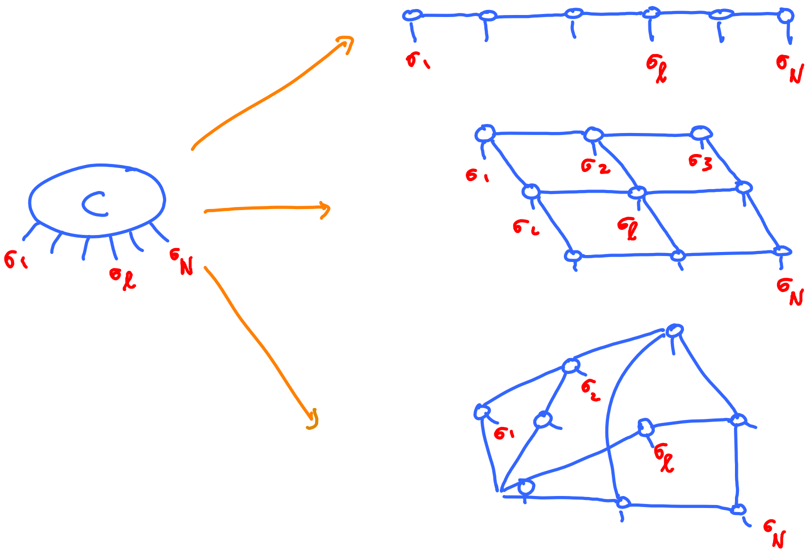
$C^{\vec{\sigma}} = C^{\sigma_1, \dots, \sigma_N}$ is a tensor of rank N (rank = number of legs)

Graphical representation: $\quad C^{\vec{\sigma}} \equiv$ (8)



one leg for each index

Claim: such a rank L tensor can be represented in many different ways:



MPS:
matrix product state

PEPS:
projected entangled-pair state

arbitrary tensor network

- a link between two sites represents entanglement between them

- different representations ⇒ different entanglement book-keeping

- tensor network = entanglement representation of a quantum state

2. Iterative Diagonalization

Consider a spin-s chain, with Hamiltonian

$$H^N = \sum_{\ell=1}^{N-1} \vec{S}_\ell \cdot \vec{S}_{\ell+1} + \sum_{\ell=1}^{N} \vec{S}_\ell \cdot \vec{h}_\ell \qquad (1)$$

local state space for site ℓ : $\quad |\sigma_\ell\rangle\ , \ \sigma_\ell = 1, .., \ d = 2s+1$

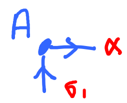
We seek eigenstates of H^N: $\quad H^N |E^N_\alpha\rangle = E^N_\alpha |E^N_\alpha\rangle\ , \quad |E^N_\alpha\rangle \in \mathcal{H}^N \qquad (2)$

$$\alpha = 1, \dots, d^N$$

Diagonalize Hamiltonian iteratively, adding one site at a time:

N=1: Start with first site, diagonalize H^1 in Hilbert space $\mathcal{H}^1$. Eigenstates have form

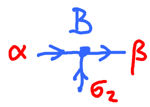
$$|\alpha\rangle \equiv |E^1_\alpha\rangle = |\sigma_1\rangle A^{\sigma_1}{}_\alpha \qquad (\alpha = 1, \dots, d) \qquad (3)$$



(sum over σ_1 implied) coefficient matrix combine 'incoming' σ_1 into 'outgoing' α

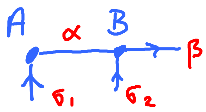
N=2: Add second site, diagonalize H^2 in Hilbert space $\mathcal{H}^2$:

$$|\beta\rangle \equiv |E^2_\beta\rangle = |\sigma_2\rangle \otimes |\alpha\rangle B^{\alpha\sigma_2}{}_\beta \qquad (\beta = 1, \dots, d^2) \qquad (4)$$



(sum over α, σ_2 implied) coefficient tensor combine 'incoming' α, σ_2 into 'outgoing' β

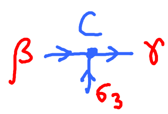
$$= \underbrace{|\sigma_2\rangle \otimes |\sigma_1\rangle}_{|\vec{\sigma}\rangle_2} A^{\sigma_1}{}_{\underbrace{\alpha\ B}}{}^{\alpha\sigma_2}{}_\beta$$



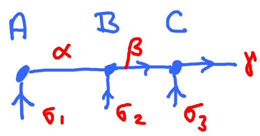
'matrix multiplication' for 'contracted' index α

N=3: Add third site, diagonalize H^3 in Hilbert space $\mathcal{H}^3$:

$$|\gamma\rangle = |\sigma_3\rangle \otimes |\beta\rangle C^{\beta\sigma_3}{}_\gamma \qquad (\gamma = 1, \dots, d^3) \qquad (5)$$



$$= \underbrace{|\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle}_{|\vec{\sigma}\rangle_3} A^{\sigma_1}{}_{\underbrace{\alpha\ B}}{}^{\alpha\sigma_2}{}_{\underbrace{\beta\ C}}{}^{\beta\sigma_3}{}_\gamma$$



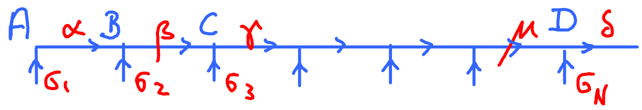
contracted indices α, β

Continue similarly until having added site N. Eigenstates of H^N in $\mathcal{H}^N$ have following structure:

$$|E^N_\delta\rangle = |\delta\rangle = |\sigma_N\rangle \otimes \dots \otimes |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle \underbrace{A^{\sigma_1}{}_\alpha B^{\alpha\sigma_2}{}_\beta C^{\beta\sigma_3}{}_\gamma \dots D^{\mu\sigma_N}{}_\delta}_{\equiv C^{\vec\sigma}{}_\delta}$$

$$= |\vec\sigma\rangle_N \, C^{\vec\sigma}{}_\delta$$ 'matrix product state' (MPS)

$(\delta = 1, \dots, d^N)$



Nomenclature: σ_ℓ = physical indices, $\alpha, \beta, \gamma, \dots$ = (virtual) bond indices

Alternative, widely-used notation: 'reshape' the coefficient tensors as

$$\tilde{A}^{\sigma_1}_{\alpha} \equiv A^{\sigma_1}{}_\alpha , \quad \tilde{B}^{\sigma_2}_{\alpha\beta} \equiv B^{\alpha\sigma_2}{}_\beta , \quad \tilde{C}^{\sigma_3}_{\beta\gamma} \equiv C^{\beta\sigma_3}{}_\gamma$$

to highlight 'matrix product' structure in noncovariant notation:

$$|\delta\rangle = |\sigma_1\rangle \otimes \dots \otimes |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle \, \tilde{A}^{\sigma_1}_{\alpha} \tilde{B}^{\sigma_2}_{\alpha\beta} \tilde{C}^{\sigma_3}_{\beta\gamma} \dots \tilde{D}^{\sigma_N}_{\mu\delta}$$

Comments

1. Iterative diagonalization of ID chain generates eigenstates whose wave functions are tensors that are expressed as matrix products.

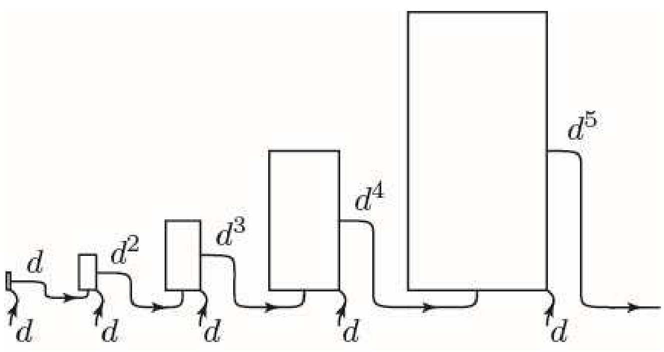
Such states an called 'matrix product states' (MPS)

Matrix size grows exponentially:

for given σ_1, $A^{\sigma_1}{}_{\alpha}$ has dimension $1 \times d$ (vector)

for given σ_2, $B^{\alpha\sigma_2}{}_{\beta}$ has dimension $d \times d^2$ (rectangular matrix)

for given σ_3, $C^{\beta\sigma_3}{}_{\gamma}$ has dimension $d^2 \times d^3$ (larger rectangular matrix)



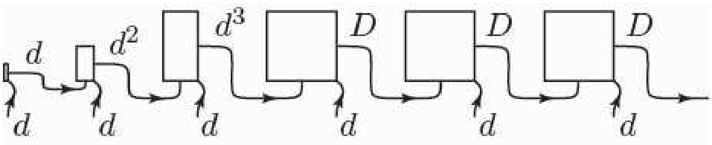
$\dots \; d^N$

"Hilbert space is a large place"

Numerical costs explode with increasing N, so truncation schemes will be needed...

Truncation can be done in controlled way using tensor network methods!

Standard truncation scheme: use $\alpha, \beta, \gamma, \ldots \leq D$ for all virtual bonds



2. Number of parameters available to encode state:

$$\mathcal{N}_{MPS} \leq N \cdot D^2 \cdot d$$

would be '=' if all virtual bonds have the same dimension, D : $\overset{D}{A}^{\mu \sigma}{}_{\lambda}$ $\sigma \sim d$, $\lambda \sim D$

$\mathcal{N}_{MPS}$ scales linearly with system size, N

If N is large: $\mathcal{N}_{MPS} \lll d^N$

Why should this have any chance of working? Remarkable fact: for 1d Hamiltonians with local interactions and a gapped spectrum, ground state can be accurately represented by MPS!

Why? 'Area laws'! Tensor Network Basics II, section 1.

3. Covariant index notation

TNB-I.3

For exposition of covariant index notation, see chapters L2 & L10 of
"Mathematics for Physicists", Altland & von Delft, www.cambridge.org/altland-vondelft

Index and arrow conventions below, adopted throughout this course, are really useful, though not (yet) standard.

Kets (Hilbert space vectors)

For kets, indices sit downstairs. E.g. basis kets: $|\varphi_\sigma\rangle$

For components of kets (w.r.t. a basis), indices sit upstairs: $|\phi\rangle = |\varphi_\sigma\rangle A^\sigma$ (1)

Repeated indices (always up-down pairs) are summed over, summation $\sum_\sigma$ is implied.

Linear combinations of kets: $\boxed{|\phi_\alpha\rangle = |\varphi_\sigma\rangle A^\sigma{}_\alpha}$ (2)

Note: for $A^\sigma{}_\alpha$ the index σ identifies components of kets, hence sits upstairs
the index α identifies basis kets (vectors), hence sits downstairs

Basis for direct product space: $|\varphi_{\vec\sigma}\rangle \equiv |\varphi_{\sigma_1\sigma_2\ldots\sigma_N}\rangle \equiv |\varphi_{\sigma_N}\rangle \otimes \ldots \otimes |\varphi_{\sigma_2}\rangle \otimes |\varphi_{\sigma_1}\rangle$ (3)

Note ket order: start with first space on very right, successively attach new spaces from the left.

Linear combinations: $|\phi_\beta\rangle = |\varphi_{\sigma_1\sigma_2\ldots\sigma_N}\rangle A^{\sigma_1\sigma_2\ldots\sigma_N}{}_\beta \equiv |\varphi_{\vec\sigma}\rangle A^{\vec\sigma}{}_\beta$ (4)

Bras (Hilbert space dual vectors)

For bras, indices sit upstairs. E.g. basis bras: $\langle\varphi^\sigma|$ (5)

For components of bras (w.r.t. a basis), indices sit downstairs: $\langle\phi| = A^\dagger{}_\sigma \langle\varphi^\sigma|$ (6)

Complex conjugation [(3) is dual of (1)]: $A^\dagger{}_\sigma = \overline{A^\sigma}$ (7)

Linear combinations of bras: $\boxed{\langle\phi^\alpha| = A^{\dagger\alpha}{}_\sigma \langle\varphi^\sigma|}$ (8)

Complex conjugation [(5) is dual of (2)]: $A^{\dagger\alpha}{}_\sigma = \overline{A^\sigma{}_\alpha}$ (Hermitian conjugation!) (9)

Note: for $A^{\dagger\alpha}{}_\sigma$, the index α identifies basis bras (dual vectors), hence sits upstairs
the index σ identifies components of bras, hence sits downstairs

Basis for direct product space: $\langle\varphi^{\vec\sigma}| \equiv \langle\varphi^{\sigma_1\sigma_2\ldots\sigma_N}| \equiv \langle\varphi^{\sigma_1}| \otimes \langle\varphi^{\sigma_2}| \otimes \ldots \otimes \langle\varphi^{\sigma_N}|$ (10)

Note bra order: opposite to that of kets in (3), so expectation values yield nested bra-ket pairs:

$$\langle\varphi^{\sigma_1\sigma_2\ldots\sigma_N}|\hat{O}|\varphi_{\sigma_1\sigma_2\ldots\sigma_N}\rangle = \langle\varphi^{\sigma_1}| \otimes \langle\varphi^{\sigma_2}| \otimes \ldots \otimes \langle\varphi^{\sigma_N}|\hat{O}|\varphi_{\sigma_N}\rangle \otimes \ldots \otimes |\varphi_{\sigma_2}\rangle \otimes |\varphi_{\sigma_1}\rangle \quad (11)$$

Linear combinations: $\langle\phi^\beta| = A^{\dagger\beta}{}_{\sigma_N\ldots\sigma_2\sigma_1} \langle\varphi^{\sigma_1\sigma_2\ldots\sigma_N}| \equiv A^{\dagger\beta}{}_{\vec\sigma_R}$ (12)
reversed index order on tensor!

Complex conjugation [(12) is dual of (4)]: $A^{\dagger\beta}{}_{\vec\sigma_R} = \overline{A^{\vec\sigma}{}_\beta}$ (Hermitian conjugation!) (13)

Orthonormality

If $\{|\varphi_\sigma\rangle\}$ form orthonormal basis: $$\langle \varphi^\sigma | \varphi_{\sigma'}\rangle = \delta^\sigma{}_{\sigma'} \tag{14}$$

If $\{|\phi_\alpha\rangle\}$ form orthonormal basis, too: $$\langle \phi^\alpha | \phi_{\alpha'}\rangle = \delta^\alpha{}_{\alpha'} \tag{15}$$

Combined: $$\delta^\alpha{}_{\alpha'} = \langle\phi^\alpha|\phi_{\alpha'}\rangle = A^{\dagger\alpha}{}_\sigma \underbrace{\langle\sigma|\sigma'\rangle}_{\delta^\sigma{}_{\sigma'}} A^{\sigma'}{}_{\alpha'} = A^{\dagger\alpha}{}_\sigma A^\sigma{}_{\alpha'} = (A^\dagger A)^\alpha{}_{\alpha'} \tag{16}$$

Hence A is unitary: $$\mathbb{1} = A^\dagger A \quad \Rightarrow \quad A^{-1} = A^\dagger \tag{17}$$

Operators $$\hat O = |\phi_{\vec\sigma}\rangle O^{\vec\sigma}{}_{\vec\sigma'}\langle\phi^{\vec\sigma'}| \,, \qquad O^{\vec\sigma}{}_{\vec\sigma'} = \langle\phi^{\vec\sigma}|\hat O|\phi_{\vec\sigma'}\rangle \tag{18}$$

Simplified notation

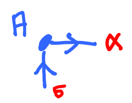
It is customary to simplify notational conventions for kets and bras:

In kets, use subscript indices as ket names: $$|\vec\sigma\rangle \equiv |\varphi_{\vec\sigma}\rangle \equiv |\sigma_1,\sigma_2,\dots,\sigma_N\rangle \equiv |\sigma_N\rangle\otimes\dots\otimes|\sigma_2\rangle\otimes|\sigma_1\rangle \tag{19}$$

In bras, use superscript indices as bra names: $$\langle\vec\sigma| \equiv \langle\varphi^{\vec\sigma}| \equiv \langle\sigma_1,\sigma_2,\dots,\sigma_N| \equiv \langle\sigma_1|\otimes\langle\sigma_2|\otimes\dots\otimes\langle\sigma_N| \tag{20}$$

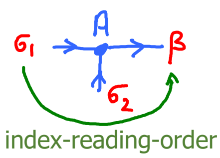
Now up/down convention for indices is no longer displayed; but it is still implicit!

Linear combination of kets: $$|\alpha\rangle \overset{(2)}{=} |\sigma\rangle A^\sigma{}_\alpha \tag{21}$$



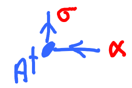
Coefficient matrix = overlap: $$A^\sigma{}_\alpha = \langle\sigma|\alpha\rangle \tag{22}$$

If direct products are involved: $$|\beta\rangle \overset{(4)}{=} |\sigma_2\rangle\otimes|\sigma_1\rangle A^{\sigma_1\sigma_2}{}_\beta \tag{23}$$



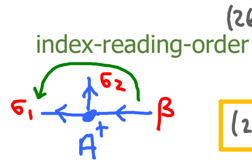
Coefficient matrix = overlap: $$A^{\sigma_1\sigma_2}{}_\beta = \langle\sigma_1|\otimes\langle\sigma_2|\beta\rangle \tag{24}$$

Linear combination of bras: $$\langle\alpha| \overset{(8)}{=} A^{\dagger\alpha}{}_\sigma\langle\sigma| \tag{25}$$



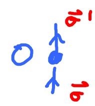
Coefficient matrix = overlap: $$A^{\dagger\alpha}{}_\sigma = \langle\alpha|\sigma\rangle = \overline{\langle\sigma|\alpha\rangle} \overset{(22)}{=} \overline{A^\sigma{}_\alpha} \tag{26}$$

If direct products are involved: $$\langle\beta| \overset{(12)}{=} A^{\dagger\beta}{}_{\sigma_2\sigma_1}\langle\sigma_1|\otimes\langle\sigma_2| \tag{27}$$



Coefficient matrix = overlap: $$A^{\dagger\beta}{}_{\sigma_2\sigma_1} = \langle\beta|\sigma_2\rangle\otimes|\sigma_1\rangle = \overline{\langle\sigma_1|\otimes\langle\sigma_2|\beta\rangle} \overset{(24)}{=} \overline{A^{\sigma_1\sigma_2}{}_\beta} \tag{28}$$

Operators: $$\hat O \overset{(18)}{=} |\vec\sigma\rangle O^{\vec\sigma}{}_{\vec\sigma'}\langle\vec\sigma'| \,, \qquad O^{\vec\sigma}{}_{\vec\sigma'} \overset{(11)}{=} \langle\vec\sigma|\hat O|\vec\sigma'\rangle \tag{29}$$



In all these overlaps (22,24,26,28):

bra indices: written upstairs on A or $A^\dagger$, depicted by incoming arrows

ket indices: written downstairs on A or $A^\dagger$, depicted by outgoing arrows

Mnemonic for arrow directions: 'airplane landing': flying in (up in air), rolling out (down on ground).