Tensor Network Basics II

TNB-II.1

1. Covariant index notation

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.

Premise: in Linear Algebra, vectors and dual vectors are notationally distinguished by lower/upper placement of indices ('covariant notation'). In Quantum Mechanics, kets are vectors, bras are dual vectors, and in the physics literature, they are distinguished by shape of brackets $|\ \rangle$ vs. $\langle\ |$. Nevertheless, it may be useful to additionally distinguish them by lower/upper placement of indices. Reason: their coefficients then inherit distinguished upper/lower index placements too, which is useful for knowing which indices can be contracted -- in particular when converting algebraic notation to tensor network notation.

In the introductory parts of this course, we will therefore use covariant notation and carefully distinguish lower/upper indices. This is not standard in QM or in the tensor network literature. But I believe that it is pedagogically useful to use notation that emphasizes vector space / dual vector space structure of QM not just for vectors / dual vectors, but also for coefficients.

Vector space, dual space (reminder)

Let $\mathbb{V}$ be a complex vector space, with elements $\psi \in \mathbb{V}$

Its dual space, $\mathbb{V}^*$, is defined as the set of all linear maps Φ of $\mathbb{V}$ to the complex numbers:

$\Phi : \mathbb{V} \to \mathbb{C}$, $\psi \to \Phi(\psi)$ with $\Phi(\psi+\psi') = \Phi(\psi) + \Phi(\psi') \quad \forall \ \psi, \psi' \in \mathbb{V}$ (1)

$\Phi(a\psi) = a\Phi(\psi) \quad \forall\ a \in \mathbb{C},\ \psi \in \mathbb{V}$ (2)

If $\mathbb{V}$ is equipped with a scalar product, $\langle , \rangle : \mathbb{V} \otimes \mathbb{V} \to \mathbb{C}$, $(\psi, \psi') \mapsto \langle \psi, \psi' \rangle$ (3)

there is a canonical identification, J, between the elements of $\mathbb{V}$ and $\mathbb{V}^*$:

$J : \mathbb{V} \to \mathbb{V}^*$, $\psi \to J(\psi) = \Psi$ such that $\Psi(\psi') = \langle \psi, \psi' \rangle \ \forall \ \psi' \in \mathbb{V}$ (4)

All properties of the map J follow directly from those of the complex scalar product s. (5)

For example, $\langle a\psi, \psi' \rangle = \bar{a} \langle \psi, \psi' \rangle$ implies that $J(a\psi) = \bar{a} J(\psi)$ (6)

ovebar denotes complex conjugation

Quantum mechanics has this vector space/ dual space structure: $\mathbb{V}$ = Hilbert space

vectors are denoted $|\psi\rangle := \psi$, dual vectors $\langle\psi| := J(|\psi\rangle)$, scalar product: $\langle\psi|\psi'\rangle := \langle\psi,\psi'\rangle$ (7)

they map vectors to complex numbers via $\langle\psi| : |\psi'\rangle \mapsto \langle\psi|\psi'\rangle$ (8)

dual vector, vector, complex number

...with $J(a|\psi\rangle) = \bar{a}\langle\psi|$, etc. (9)

they map vectors to complex numbers via $\langle\psi|$: $|\psi'\rangle \mapsto \langle\psi|\psi'\rangle$ (8)

dual vector — vector — complex number

with $J(a|\psi\rangle) = \bar{a}\langle\psi|$, etc. (9)

Therefore, covariant index notation for vectors/dual vectors can also be used for kets/bras, as follows:

Vectors (kets)

Indices labeling vectors (kets) sit downstairs. E.g. basis kets: $|\varphi_\sigma\rangle \in \mathbb{V}$ (10) ~ vector space

Indices labeling components of vectors (kets) sit upstairs: $|\phi\rangle = |\varphi_\sigma\rangle A^\sigma \in \mathbb{V}$ (11)

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

Indices labeling linear combinations of kets sit downstairs: $|\phi_\alpha\rangle = \boxed{|\varphi_\sigma\rangle A^\sigma{}_\alpha} \in \mathbb{V}$ (12)

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

Dual vectors (bras)

Indices labeling dual vectors (bras) sit upstairs. E.g. basis bras: $\langle\varphi^\sigma| \in \mathbb{V}^*$ (13) ~ dual space

Indices labeling components of dual vectors (bras) sit downstairs: $\langle\phi| \overset{(11)}{=} \bar{A}^\sigma\langle\varphi^\sigma| \overset{(15)}{=} \boxed{A^\dagger{}_\sigma\langle\varphi^\sigma|}$ (14)

Complex conjugation [(14) is dual of (11)]: $A^\dagger{}_\sigma \overset{\text{definition}}{:=} \bar{A}^\sigma$ (15)

Indices labeling linear combination of kets sit upstairs: $\langle\phi^\alpha| = \overline{A^\sigma{}_\alpha}\langle\varphi^\sigma| = \boxed{A^{\dagger\alpha}{}_\sigma\langle\varphi^\sigma|}$ (16)

Complex conjugation [(16) is dual of (12)]: $A^{\dagger\alpha}{}_\sigma \overset{\text{definition}}{:=} \overline{A^\sigma{}_\alpha}$ (Hermitian conjugation!) (17)

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

Overlaps

Suppose $\{|\varphi_\sigma\rangle\}$ form orthonormal basis:

$\langle\varphi^\sigma|\varphi_{\sigma'}\rangle = \delta^\sigma{}_{\sigma'}$

$\langle\varphi^\sigma|\phi_{\alpha'}\rangle = \underbrace{\langle\varphi^\sigma|\varphi_{\sigma'}\rangle}_{\delta^\sigma{}_{\sigma'}} A^{\sigma'}{}_{\alpha'} = A^\sigma{}_{\alpha'}$

$\langle\phi^\alpha|\varphi_{\sigma'}\rangle = A^{\dagger\alpha}{}_\sigma\langle\varphi^\sigma|\varphi_{\sigma'}\rangle = A^{\dagger\alpha}{}_{\sigma'}$

$\langle\phi^\alpha|\phi_{\alpha'}\rangle = A^{\dagger\alpha}{}_\sigma A^\sigma{}_{\alpha'} = (A^\dagger A)^\alpha{}_{\alpha'}$

Linear algebra perspective

dual vector maps vector to number

$\langle\varphi^\sigma| : |\varphi_{\sigma'}\rangle \mapsto \delta^\sigma{}_{\sigma'}$ (18)

$\langle\varphi^\sigma| : |\phi_{\alpha'}\rangle \mapsto A^\sigma{}_{\alpha'}$ (19)

$\langle\phi^\alpha| : |\varphi_{\sigma'}\rangle \mapsto A^{\dagger\alpha}{}_{\sigma'}$ (20)

$\langle\phi^\alpha| : |\phi_{\alpha'}\rangle \mapsto (A^\dagger A)^\alpha{}_{\alpha'}$ (21)

Unitarity

Unitarity

Suppose that $\{|\phi_\alpha\rangle\}$ form orthonormal basis, too: $\langle\phi^\alpha|\phi_{\alpha'}\rangle = \delta^\alpha{}_{\alpha'}$ (22)

Combined: $\delta^\alpha{}_{\alpha'} = \langle\phi^\alpha|\phi_{\alpha'}\rangle = A^{\dagger\alpha}{}_\sigma \underbrace{\langle\varphi_\sigma|\varphi_{\sigma'}\rangle}_{\delta_{\sigma\sigma'}} A^{\sigma'}{}_{\alpha'} = A^{\dagger\alpha}{}_\sigma A^\sigma{}_{\alpha'} = (A^\dagger A)^\alpha{}_{\alpha'}$ (23)

Hence A is unitary: $\mathbb{1} = A^\dagger A \quad\Rightarrow\quad A^{-1} = A^\dagger$ (24)

$\Longrightarrow$ Two orthonormal bases are related by a unitary transformation.

Completeness $\mathbb{1} = |\varphi_\sigma\rangle\langle\varphi^\sigma| = |\phi_\alpha\rangle\langle\phi^\alpha|$ (25)

Operators $\hat{O} = |\varphi_{\sigma'}\rangle\langle\varphi^{\sigma'}|\hat{O}|\varphi_\sigma\rangle\langle\varphi^\sigma| = |\varphi_{\sigma'}\rangle \underbrace{O^{\sigma'}{}_\sigma}_{:=} \langle\varphi^\sigma|$ (26)

Covariant notation works nicely! So why is it not commonly used in quantum mechanics?

For orthonormal basis, the 'metric' is trivial: $\langle\varphi^\sigma|\varphi_{\sigma'}\rangle = \delta^\sigma{}_{\sigma'}$ (27)

Therefore , index raising and lowering using metric does not change numerical value of object:

raising: $|\varphi^\sigma\rangle = \delta^{\sigma\sigma'}|\varphi_{\sigma'}\rangle = |\varphi_\sigma\rangle$, lowering: $\langle\varphi_{\sigma'}| = \langle\varphi^\sigma|\delta_{\sigma\sigma'} = \langle\varphi^{\sigma'}|$ (28)

In quantum mechanics, we can always choose an orthonormal basis, so that metric is trivial, and then it is not necessary to distinguish between upper/lower indices. Hence this is typically not done in QM literature.

Nevertheless, for tensor networks, the position (upstairs/downstairs) of a tensor index does carry useful information: it reminds us that the tensor carrying the index is a coefficient of a ket (a vector) or bra (a dual vector) respectively. In other words, index positions on tensors carry structure-revealing information that is not kept track of in bra-ket information. (There, structural information is carried in the notation for states, $|\psi\rangle$ vs. $\langle\varphi|$, but not for their coefficients).

When drawing tensor network diagrams for many-particle systems, this information is a useful guide for keeping track of allowed contractions: only upper with lower index!

2. Arrow conventions

For systems involving many tensors, e.g. many-particle systems, it is useful to visualized covariant notation via arrows on tensor legs. Consider lattice with $\mathcal{L}$ sites.

Kets: direct product basis: $|\varphi_{\vec{\sigma}}\rangle \equiv |\varphi_{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}\rangle \equiv |\varphi_{\sigma_1}\rangle\otimes|\varphi_{\sigma_2}\rangle\otimes\ldots\otimes|\varphi_{\sigma_{\mathcal{L}}}\rangle \in \mathbb{V}^{\mathcal{L}}$ (1)

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

Linear combinations: $|\phi_\beta\rangle = |\varphi_{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}\rangle A^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}{}_\beta =: |\varphi_{\vec{\sigma}}\rangle A^{\vec{\sigma}}{}_\beta \in \mathbb{V}^{\mathcal{L}}$ (2)

Bras: direct product space: $\langle\varphi^{\vec{\sigma}}| := \langle\varphi^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}| := \langle\varphi^{\sigma_{\mathcal{L}}}|\otimes\ldots\otimes\langle\varphi^{\sigma_2}|\otimes\langle\varphi^{\sigma_1}| \in \mathbb{V}^{*\mathcal{L}}$ (3)

Note bra order: opposite to that of kets in (1), so expectation values yield nested bra-ket pairs:

$$\langle\varphi^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}|\hat{O}|\varphi_{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}\rangle = \langle\varphi^{\sigma_{\mathcal{L}}}|\otimes\ldots\otimes\langle\varphi^{\sigma_2}|\otimes\langle\varphi^{\sigma_1}|\hat{O}|\varphi_{\sigma_1}\rangle\otimes|\varphi_{\sigma_2}\rangle\otimes\ldots\otimes|\varphi_{\sigma_{\mathcal{L}}}\rangle \quad (4)$$

Linear combinations: $\langle\phi^\beta| = \overline{A^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}{}_\beta}\,\langle\varphi^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}|$ (5)

Complex conjugation: (5) is dual of (2)
$= A^{\dagger\beta}{}_{\sigma_{\mathcal{L}}\ldots\sigma_2\sigma_1}\langle\varphi^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}| = A^{\dagger\beta}{}_{\vec{\sigma}_R}\langle\varphi^{\vec{\sigma}}|$ (6)

Definition of meaning of $\dagger$: ('generalized Hermitian conjugation'):
$A^{\dagger\beta}{}_{\vec{\sigma}_R} = A^{\dagger\beta}{}_{\sigma_{\mathcal{L}}\ldots\sigma_2\sigma_1} := \overline{A^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}{}_\beta} =: \overline{A^{\vec{\sigma}}}{}_\beta$ (7)

convention: index order on tensor is reversed (R) from that on bra indices

Overlap: $\langle\phi^{\beta'}|\phi_\beta\rangle \overset{(2,5)}{=} A^{\dagger\beta'}{}_{\vec{\sigma}_R}\langle\varphi^{\vec{\sigma}'}|\varphi_{\vec{\sigma}}\rangle A^{\vec{\sigma}}{}_\beta = A^{\dagger\beta'}{}_{\vec{\sigma}_R}A^{\vec{\sigma}}{}_\beta$ (8)

$\overset{(6)}{=} A^{\dagger\beta}{}_{\sigma_{\mathcal{L}}\ldots\sigma_2\sigma_1}A^{\sigma_1\sigma_2\ldots\sigma_{\mathcal{L}}}{}_\beta$ (9)

achieving this nested contraction pattern is motivation for definition of $A^\dagger$ in (6)

Easy to remember: 'contract each index with its dual partner' !

Simplified notation

It is customary to simplify notational conventions for kets and bras (don't write φ, ϕ so often):

In kets, use subscript indices as ket names: $|\vec{\sigma}\rangle := |\sigma_1,\sigma_2,\ldots,\sigma_{\mathcal{L}}\rangle = |\sigma_1\rangle\otimes|\sigma_2\rangle\otimes\ldots\otimes|\sigma_{\mathcal{L}}\rangle$ (10)

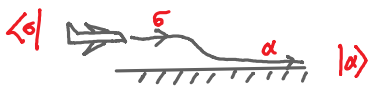
In bras, use superscript indices as bra names: $\langle\vec{\sigma}| := \langle\sigma_1,\sigma_2,\ldots,\sigma_{\mathcal{L}}| := \langle\sigma_{\mathcal{L}}|\otimes\ldots\otimes\langle\sigma_2|\otimes\langle\sigma_1|$ (11)

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

Proliferation of indices calls for graphical notation!

Index positions (upstairs / downstairs) on <u>tensors</u> will be depicted by arrows (incoming / outgoing):

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



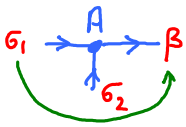
(TNB-II.1.12)

Linear combination of kets: $|\alpha\rangle = |\sigma\rangle A^{\sigma}{}_{\alpha}$ (12)

Coefficient matrix = overlap: $A^{\sigma}{}_{\alpha} = \langle\sigma|\alpha\rangle$ (13)

(TNB-II.2.2)

If direct products are involved: $|\beta\rangle = |\sigma_1\rangle\otimes|\sigma_2\rangle A^{\sigma_1\sigma_2}{}_{\beta}$ (14)



Coefficient matrix = overlap: $A^{\sigma_1\sigma_2}{}_{\beta} = \langle\sigma_2|\otimes\langle\sigma_1|\beta\rangle$ (15)

index-reading order

(TNB-II.1.16)

Linear combination of bras: $\langle\alpha| = A^{\dagger\alpha}{}_{\sigma}\langle\sigma|$ (16)

Coefficient matrix = overlap: $A^{\dagger\alpha}{}_{\sigma} = \langle\alpha|\sigma\rangle = \overline{\langle\sigma|\alpha\rangle} \overset{(11)}{=} \overline{A^{\sigma}{}_{\alpha}}$ (17)

index-reading order

(TNB-II.2.7)

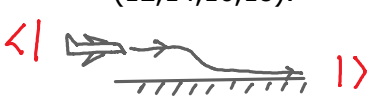
If direct products are involved: $\langle\beta| = A^{\dagger\beta}{}_{\sigma_2\sigma_1}\langle\sigma_2|\otimes\langle\sigma_1|$ (18)

Coefficient matrix = overlap: $A^{\dagger\beta}{}_{\sigma_2\sigma_1} = \langle\beta|\sigma_1\rangle\otimes|\sigma_2\rangle = \overline{\langle\sigma_2|\otimes\langle\sigma_1|\beta\rangle} \overset{(15)}{=} \overline{A^{\sigma_1\sigma_2}{}_{\beta}}$ (19)

(TNB-II.1.26)

Operators: $\hat{O} = |\vec{\sigma}'\rangle O^{\vec{\sigma}'}{}_{\vec{\sigma}}\langle\vec{\sigma}|$, $O^{\vec{\sigma}'}{}_{\vec{\sigma}} = \langle\vec{\sigma}'|\hat{O}|\vec{\sigma}\rangle$ (20)

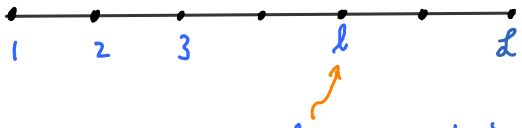
In all these overlaps (12,14,16,18):



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

3. Iterative diagonalization [generates a 1d tensor network]

Consider a spin-s chain, with Hamiltonian $H^{\ell} = J \sum_{\ell=1}^{\ell-1} \vec{S}_\ell \cdot \vec{S}_{\ell+1} + \sum_{\ell=1}^{\ell} \vec{S}_\ell \cdot \vec{h}_\ell$ (1)



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

We seek eigenstates of H^{ℓ} : $H^{\ell} |E^{\ell}_\alpha\rangle = E^{\ell}_\alpha |E^{\ell}_\alpha\rangle$, $|E^{\ell}_\alpha\rangle \in \mathcal{H}^{\ell}$ (2)

$\alpha = 1, \dots, d$

Diagonalize Hamiltonian iteratively, adding one site at a time:

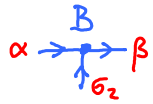
ℓ =1: Start with first site, diagonalize H^1 in Hilbert space $\mathcal{H}^1$. Eigenstates have form

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

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

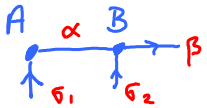
ℓ =2: Add second site, diagonalize H^2 in Hilbert space $\mathcal{H}^2$:

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



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

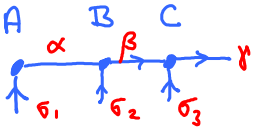
$$= \underbrace{|\sigma_1\rangle \otimes |\sigma_2\rangle}_{|\vec{\sigma}\rangle_2} A^{\sigma_1}{}_\alpha \underbrace{B^{\alpha\sigma_2}{}_\beta}_{\text{'matrix multiplication' for 'contracted' index } \alpha}$$



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

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

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



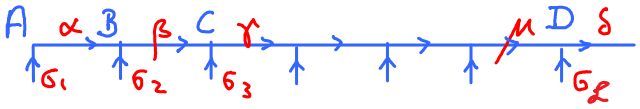
contracted indices α, β

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

$|E^{\ell}_{\delta}\rangle = |\delta\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes |\sigma_3\rangle \otimes \dots \otimes |\sigma_\ell\rangle \; \underbrace{A^{\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta} C^{\beta\sigma_3}{}_{\gamma} \dots D^{\mu\sigma_\ell}{}_{\delta}}_{:= C^{\vec{\sigma}}{}_{\delta}}$

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

$(\delta = 1, \dots, d^{\ell})$



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

Alternative, widely-used notation: 'reshape' the coefficient tensors, such that physical indices are all upstairs, others all downstairs:

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

to highlight 'matrix product' structure in noncovariant notation:

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

Comments

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

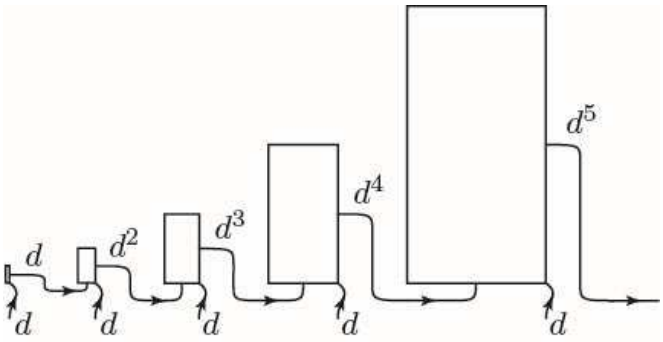
Such states an called 'matrix product states' (MPS)

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)

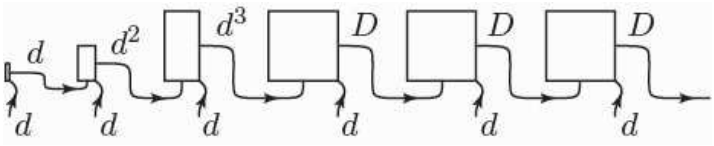


'Hilbert space is a large place'

Numerical costs increase exponentially with increasing $\mathcal{L}$, 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:

$N_{MPS} \leq \mathcal{L} \cdot D^2 \cdot d$

would be '=' if all virtual bonds have the same dimension, D :

$D_\lambda \sim d$

$A^{\mu}{}_{\sigma\lambda} \sim D$

N_{MPS} scales linearly with system size, $\mathcal{L}$

If $\mathcal{L}$ is large: $N_{MPS} \ll d^{\mathcal{L}}$

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'! (TNB-1.2)