A numerical introduction to tensor networks for quantum simulation

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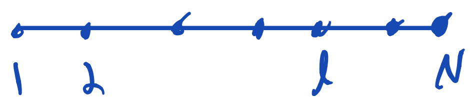
[Credit for course materials: Prof. Jan von Delft]

1. Why tensor networks?

Tensor networks provide a flexible description of quantum states.

In some cases, they are efficient - can accurately describe state with polynomial resources.

Example: spin- s chain, with N sites:



Local state space of site ℓ : $|\sigma_\ell\rangle_\ell \in \{|1\rangle_\ell, |2\rangle_\ell, \ldots, |2s+1\rangle_\ell\}$

Local state label: $\sigma = 1, 2, \ldots 2s+1$

Local dimension: $d \equiv 2s+1$

Shorthand: $|\sigma_\ell\rangle \equiv |\sigma_\ell\rangle_\ell$

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

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

$$|\sigma_N\rangle \otimes \cdots \otimes |\sigma_\ell\rangle \otimes \ldots \otimes |\sigma_1\rangle \equiv |\sigma_1, \sigma_2 \ldots \sigma_N\rangle$$
$$\equiv |\bar{\sigma}\rangle_N$$

Hilbert space for full chain: $\mathcal{H}^N = \text{span}(\{|\bar{\sigma}\rangle_N\})$ ← superpositions

Generic quantum state: $(\in \mathcal{H}^N)$ $|\psi\rangle_N = \sum_{\sigma_1 \ldots \sigma_N} |\sigma_1 \ldots \sigma_N\rangle C^{\sigma_1 \ldots \sigma_N} \equiv \underbrace{C^{\bar{\sigma}} |\bar{\sigma}\rangle_N}_{\text{summation implied}}$

Dimension of full Hilbert space $\mathcal{H}^N$: $\underbrace{d^N}_{\text{exponential explosion}}$ (# of different configurations of $\bar{\sigma}$)

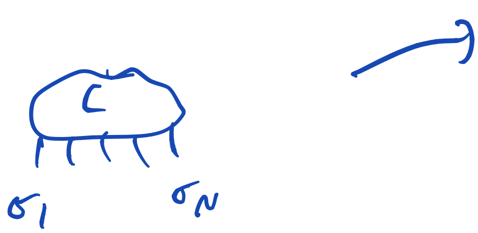
Specifying $|\psi\rangle_N$ involves specifying $C^{\bar{\sigma}}$, i.e. d^N different complex numbers.

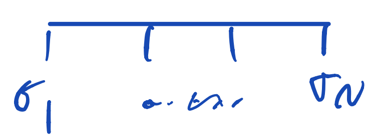
$C^{\bar{\sigma}} = C^{\sigma_1 \ldots \sigma_N}$ is a tensor of rank N (rank = # of legs)

Graphical representation: (one leg for each index)

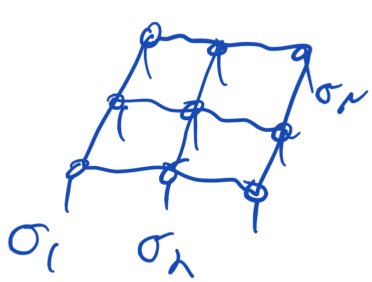
$C^{\bar{\sigma}} \equiv$

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

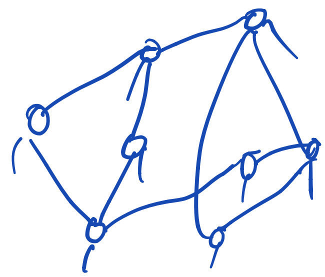




MPS: matrix product state



PEPS: projected entangled-pair state



arbitrary tensor network

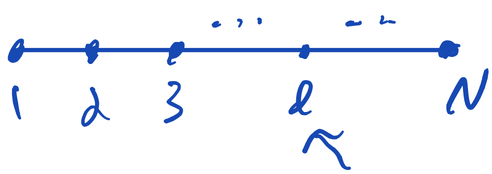
-a link between two sites represents entanglement between them — virtual indices

-different representations -> different entanglement book-keeping

-tensor network = entanglement representation of a quantum state

<u>2. Iterative diagonalization</u>

Consider a spin-s chain with Hamiltonian
$$H^N = \sum_{l=1}^{N-1} \vec{S}_l \cdot \vec{S}_{l+1} + \sum_{l=1}^{N} \vec{S}_l \cdot \vec{h}_l$$
(example)



local state space for site l : $|\sigma_l\rangle = 1, 2 \ldots d = 2s+1$

We seek eigenstates of H^N : $H^N |E_\alpha^N\rangle = E_\alpha^N |E_\alpha^N\rangle$

$|E_\alpha^N\rangle$ = eigenvector of H^N

E_α^N = eigenvalue

$|E_\alpha^N\rangle \in \mathcal{H}^N$; $\alpha = 1 \ldots d^N$

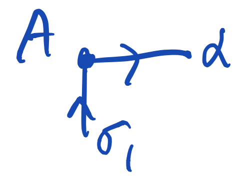
Diagonalize Hamiltonian iteratively, adding one site at a time.

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

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

σ_1 ← rows

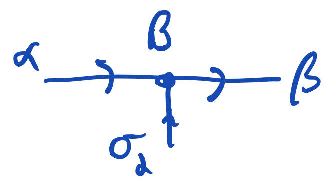
α ← columns



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

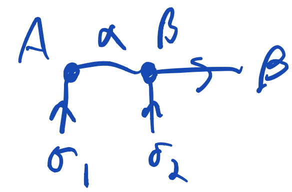
N = 2: Add second site, diagonalize H^2 in Hilbert space $\mathcal{H}^2$:

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



(sum over α,σ_2 implied) coefficient ~~matrix~~ tensor combining 'incoming' α,σ_2 into 'outgoing' β

$$|\beta\rangle = |\sigma_2\rangle \otimes |\sigma_1\rangle \underbrace{A^{\sigma_1}_{\alpha} B^{\alpha\sigma_2}}_{\text{contraction} \Leftrightarrow \text{matrix multiplication}}{}_{\beta}$$



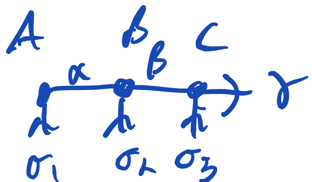
N = 3: Add third site, diagonalize H^3 in Hilbert space $\mathcal{H}^3$:

Your try:

Answer: $|\gamma\rangle = |\sigma_3\rangle \otimes |\beta\rangle\, C^{\beta\sigma_3}{}_{\gamma}$ $(\gamma = 1 \ldots d^3)$

$$= |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle\, A^{\sigma_1}{}_{\alpha}\, B^{\alpha\sigma_2}{}_{\beta}\, C^{\beta\sigma_3}{}_{\gamma}$$

Contracted

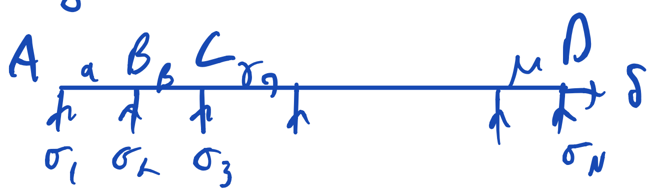


Continue similarly until having added site N. Eigenstates of H^N have following structure:

$$|E^N_\delta\rangle = |\delta\rangle = |\sigma_N\rangle \otimes \cdots \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle\, \underbrace{A^{\sigma_1}{}_{\alpha}\, B^{\alpha\sigma_2}{}_{\beta} \cdots D^{\mu\sigma_N}{}_{\delta}}_{C^{\bar{\sigma}}{}_{\delta}}$$

$$= |\bar{\sigma}_N\rangle\, C^{\bar{\sigma}}{}_{\delta} \quad \text{(MPS)}$$

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



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

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

$$\tilde{A}^{\sigma_1}_{\alpha} \equiv A^{\sigma_1}{}_{\alpha} \quad ; \quad \tilde{B}^{\sigma_2}_{\alpha\beta} \equiv B^{\alpha\sigma_2}{}_{\beta}$$

to highlight 'matrix product' structure in noncovariant notation:

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

Comments

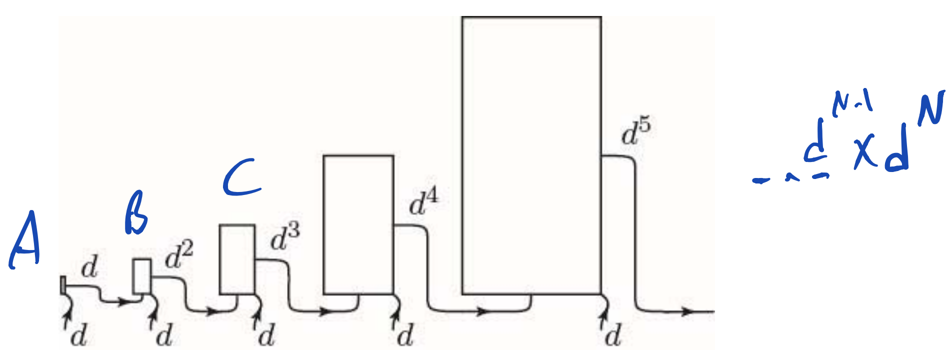
1. Iterative diagonalization of 1D chain generates eigenstates whose wave functions are tensors that are expressed as matrix products -> matrix product states (MPS)

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)

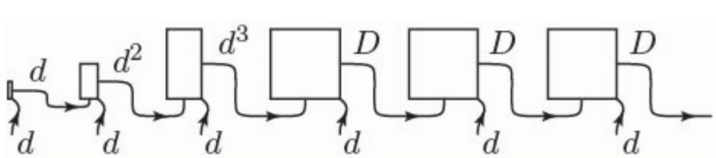


"Hilbert space is a large place!"

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

Truncation can be done in a 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:

$$A^{\overset{D}{\mu}\,\overset{d}{\sigma}\,\underset{D}{x}}$$

$$N_{MPS} \underset{\text{= if all virtual bonds have dim. } D}{\leq} N \cdot D^2 \cdot d$$

[equal if all virtual bonds have same dimension D]

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

Why should we expect this ansatz with polynomial parameters to accurately represent a quantum state?

Remarkable fact: for 1d Hamiltonian with local interactions and a gapped spectrum, its ground state can be accurately represented by MPS! $\underbrace{E_1 - E_0 > \delta \text{ as } N \to \infty}$

Reason: Area law for entanglement entropy. We will discuss later.

3. Covariant index notation

More detail of covariant index notation is in L2 & L10 of "Mathematics for Physicists", Altland & von Delft, see here.

Kets (Hilbert space vectors)

For kets, indices are down. E.g. basis kets: $|\phi_\sigma\rangle$

convention

down

For components of kets (wrt a basis), indices are upper: $|\psi\rangle = |\phi_\sigma\rangle A^\sigma$

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

Example: linear combination of kets.

Your try:

Answer: $|\psi_\alpha\rangle = |\phi_\sigma\rangle A^\sigma_{\ \alpha}$

produce a ket

Note: for $A^\sigma_{\ \alpha}$ the index σ identifies components of kets -> upper

the index α identifies components of basis kets -> lower

Basis for direct product space: $|\phi_{\bar\sigma}\rangle \equiv |\phi_{\sigma_1 \ldots \sigma_N}\rangle \equiv |\phi_N\rangle \otimes \ldots \otimes |\phi_1\rangle$

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

Linear combinations: $|\psi_\beta\rangle = |\phi_{\sigma_1 \ldots \sigma_N}\rangle A^{\sigma_1 \ldots \sigma_N}{}_{\beta}$

Your try:

$$= |\phi_{\bar\sigma}\rangle A^{\bar\sigma}{}_{\beta}$$

Answer:

<u>Bras</u> (Hilbert space <u>dual vectors</u>)

For bras, indices are upper. E.g. basis bras: $\langle\phi^\sigma|$

For components of bras (wrt a basis), indices are lower:

$$\langle\psi| = A^{\dagger}_{\sigma} \langle\phi^\sigma|$$

Complex conjugation: $A^{\dagger}_{\sigma} = \overline{A}^{\sigma}$ complex conjugation

Linear combinations of bras: $\langle \phi^{\alpha} | = A^{\dagger\alpha}_{\ \sigma} \langle \phi^{\sigma} |$

Your try:

Answer:

Complex conjugation: $A^{\dagger\alpha}_{\ \sigma} = \overline{A^{\sigma}_{\ \alpha}}$ (Hermitian conjugate)

Note: for $A^{\dagger\alpha}_{\ \sigma}$, the index α identifies basis bras (dual vectors) hence upper (out)

the index σ identifies components of bras (dual vectors) hence lower

Basis for direct product space: $\langle \phi^{\bar{\sigma}} | \equiv \langle \phi^{\sigma_1 \ldots \sigma_N} | \equiv \underbrace{\langle \phi^{\sigma_1} | \otimes \ldots \otimes \langle \phi^{\sigma_N} |}_{\text{opposite order}}$

Note bra order: opposite to kets so expectation values yield nested bra-ket pairs:

$$\langle \phi^{\sigma_1 \ldots \sigma_N} | \tilde{O} | \phi_{\sigma_1 \ldots \sigma_N} \rangle$$

$$= \langle \phi^{\sigma_1} | \otimes \ldots \langle \phi^{\sigma_N} | \hat{O} | \phi^{\sigma_N} \rangle \otimes \ldots \otimes | \sigma_1 \rangle$$

overlap now yields nested pairs

Linear combinations:
$$\langle \psi^\beta | = A^{\dagger\beta}{}_{\underbrace{\sigma_N\cdots\sigma_1}_{\text{reversed index order}}} \langle \phi^{\sigma_1\cdots\sigma_N}| = A^{\dagger\beta}{}_{\bar\sigma}\langle\phi^{\bar\sigma}|$$

Complex conjugation:
$$A^{\dagger\beta}{}_{\bar\sigma} = \overline{A^{\bar\sigma}{}_{\beta}}$$

Orthonormality

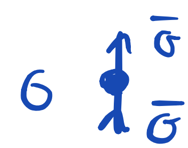
If $|\phi_\sigma\rangle$ form orthonormal basis: $\langle\phi^\sigma|\phi_{\sigma'}\rangle = \delta^{\sigma}{}_{\sigma'}$

If $|\psi_\sigma\rangle$ form orthonormal basis, too: $\langle\psi^\alpha|\psi_{\alpha'}\rangle = \delta^{\alpha}{}_{\alpha'}$

Combined:
$$\delta^{\alpha}{}_{\alpha'} = \langle\psi^\alpha|\psi_{\alpha'}\rangle = A^{\dagger\alpha}{}_{\sigma}\underbrace{\langle\sigma|\sigma'\rangle}_{\delta^{\sigma}{}_{\sigma'}} A^{\sigma'}{}_{\alpha'}$$
$$= A^{\dagger\alpha}{}_{\sigma} A^{\sigma}{}_{\alpha'} = (A^\dagger A)^{\alpha}{}_{\alpha'}$$

Hence A is unitary:
$$I = A^\dagger A \Rightarrow A^{-1} = A^\dagger$$

Operators
$$\hat{O} = |\phi_{\bar\sigma}\rangle O^{\bar\sigma}{}_{\bar\sigma'}\langle\phi^{\bar\sigma'}|$$
$$O^{\bar\sigma}{}_{\bar\sigma'} = \langle\bar\sigma|\hat{O}|\bar\sigma'\rangle$$



bra indices:
A or $A^\dagger$: up indices
incoming arrows

ket indices
A or $A^\dagger$: down
outgoing arrows

Simplified notation

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

In kets, use subscript indices as ket names: $|\phi_{\bar{\sigma}}\rangle \equiv |\bar{\sigma}\rangle \equiv |\sigma_1, \sigma_2 \ldots \sigma_N\rangle$

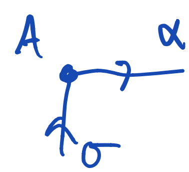
$$\equiv |\sigma_N\rangle \otimes \ldots \otimes |\sigma_1\rangle$$

In bras, use superscript indices as bra names:

$$\langle \phi^{\bar{\sigma}}| \equiv \langle \bar{\sigma}| \equiv \langle \sigma_1, \sigma_2 \ldots \sigma_N| \equiv \langle \sigma_1| \otimes \langle \sigma_2| \otimes \ldots \otimes \langle \sigma_N|$$

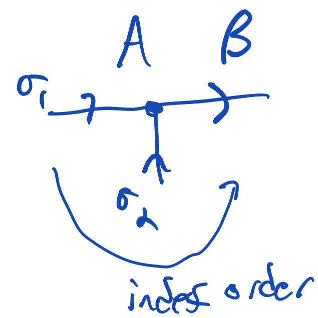
Now up/down convention for indices is no longer displayed but it still implicit!

Linear combination of kets: $|\alpha\rangle = |\sigma\rangle A^{\overset{\text{bra index}}{\sigma}}_{\underset{\text{ket index}}{\alpha}}$



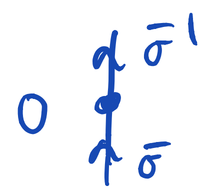
Coefficient matrix = overlap: $A^{\sigma}_{\alpha} = \langle \sigma | \alpha \rangle$

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



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

Operators: $\hat{O} = |\bar{\sigma}\rangle O^{\bar{\sigma}}_{\bar{\sigma}'} \langle \bar{\sigma}'|$



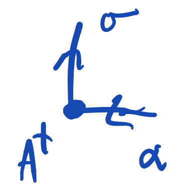
$$O^{\bar{\sigma}}_{\bar{\sigma}'} = \langle \bar{\sigma} | \hat{O} | \bar{\sigma}' \rangle$$

In the overlaps:

bra indices: upper on A or $A^\dagger$, as incoming arrows

ket indices: lower on A or $A^\dagger$, as outgoing arrows

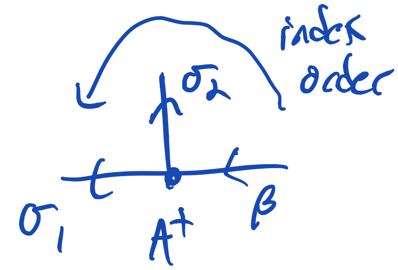
Linear combo of bras: $\langle\alpha| = A^{\dagger\alpha}{}_{\sigma}\langle\sigma|$



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

$= \overline{\langle\sigma|\alpha\rangle} = \overline{A^{\sigma}{}_{\alpha}}$ (Hermitian conjugate)

Direct products: $\langle\beta| = A^{\dagger\beta}{}_{\sigma_2\sigma_1}\langle\sigma_1|\otimes\langle\sigma_2|$

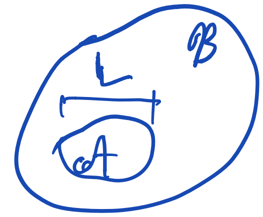


Coefficient matrix: $A^{\dagger\beta}{}_{\sigma_2\sigma_1} = \langle\beta|\sigma_2\rangle\otimes|\sigma_1\rangle$

$= \overline{\langle\sigma_1|\otimes\langle\sigma_2|\beta\rangle} = \overline{A^{\sigma_1\sigma_2}{}_{\beta}}$

4. Entanglement entropy and Area Laws (introductory comments)

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



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

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

'reduced density matrix' for $\mathcal{A}$: $\hat{\rho}_A \equiv \mathrm{Tr}_{\mathcal{B}}\, \hat{\rho}$ $\left(\hat{\rho}_{\mathcal{B}} \equiv \mathrm{Tr}_{\mathcal{A}}\, \hat{\rho} \right)$

'Entanglement entropy' of $\mathcal{A}$ and $\mathcal{B}$:

$$S_{A|B} = -\mathrm{tr}_A\, \hat{\rho}_A \log_2 \hat{\rho}_A = -\sum_\alpha w_\alpha \log_2 w_\alpha$$

w_α: eigenvalues of ρ_A

Key result: for Hamiltonians with only local interactions, $S_{A|B}$ is governed by an 'area law':

$S \equiv S_{A|B} \sim$ (area of boundary of $\mathcal{A}$) $\equiv \partial\mathcal{A}$

$\sim L^2$ in 3D for gapped system

$\sim L$ in 2D for gapped system

$\sim \text{const}$ in 1D for gapped system

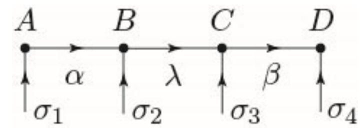
In TDL, $E_1 - E_0 > 0$

$\sim \text{const} + \ln L$ in 1D for *gapless system

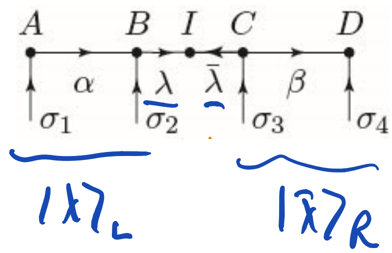
Excited states?

Now consider an MPS of maximal bond dimension D:

$$|\psi\rangle = |\sigma_4\rangle \otimes |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle A^{\sigma_1}_{\alpha} B^{\alpha\sigma_2}_{\lambda} \underbrace{C^{\lambda\sigma_3}_{\beta}}_{= I^{\lambda\bar\lambda} C^{\sigma_3}_{\bar\lambda\beta}} D^{\beta\sigma_4}$$



Divide system into two parts: $\underbrace{\text{Left -> 2 sites}}_{A}$, $\underbrace{\text{Right -> 2 sites}}_{B}$



$$|\psi\rangle = I^{\lambda\bar\lambda} |\sigma_4\rangle \otimes |\sigma_3\rangle C^{\sigma_3}_{\bar\lambda\beta} D^{\beta\sigma_4}$$
$$\otimes |\sigma_2\rangle \otimes |\sigma_1\rangle A^{\sigma_1}_{\alpha} B^{\alpha\sigma_2}_{\lambda}$$
$$= \sum_{\lambda=1}^{D} \underbrace{I^{\lambda\bar\lambda}}_{\text{implicit sum over } \bar\lambda} |\bar\lambda\rangle_R \otimes |\lambda\rangle_L$$

=entangled superposition of two state spaces, each having dimension of at most D

$$= \sum_{\lambda=1}^{D} |\lambda_R\rangle \otimes |\lambda_L\rangle$$

(After the sum over $\bar\lambda$ has been performed explicitly using Kronecker delta, result contains non-covariantly paired indices

Density matrix: $$\hat\rho = |\psi\rangle\langle\psi| = \sum_{\lambda\lambda'} |\lambda\rangle_R |\lambda\rangle_L \, {}_L\langle\lambda'| \, {}_R\langle\lambda'|$$

Reduced density matrix: $$\hat\rho_A = \mathrm{Tr}_B\,\hat\rho = \sum_{\mu} {}_R\langle\mu| \sum_{\lambda\lambda'} |\lambda\rangle_R |\lambda\rangle_L \, {}_L\langle\lambda'| \, {}_R\langle\lambda'|\mu\rangle_R$$
$$= \sum_{\lambda\lambda'} |\lambda\rangle_L (\rho_A)^{\lambda}{}_{\lambda'} \, {}_L\langle\lambda'|$$

complete set of states
$$I_B = \sum_{\mu} |\mu\rangle_R \, {}_R\langle\mu|$$

with matrix elements $(\rho_A)^{\lambda}_{\lambda'} = \sum_{\mu} {}_R\underbrace{\langle\mu|\lambda\rangle}_{\#}{}_R \; {}_R\underbrace{\langle\lambda'|\mu\rangle}_{\#}{}_R = \sum_{\mu} {}_R\langle\lambda'|\underbrace{\mu\rangle\langle\mu}_{I}|\lambda\rangle_R$

$= {}_R\langle\lambda'|\lambda\rangle = D \times D$ matrix

This matrix has rank $\leq D$ (say D)

Let w_α be its eigenvalues, with $\alpha = 1, \dots, D$

and normalization $1 = \mathrm{Tr}\,\hat{\rho}_A = \sum_\alpha w_\alpha$

Entanglement entropy: $S = -\sum_{\alpha=1}^{D} w_\alpha \log_2 w_\alpha$

Maximal if $w_\alpha = \frac{1}{D}$ for all α : $\underline{S \leq -\sum_{\alpha=1}^{D} \frac{1}{D} \log_2 \frac{1}{D} = \log_2 D}$

$2^S \leq D$

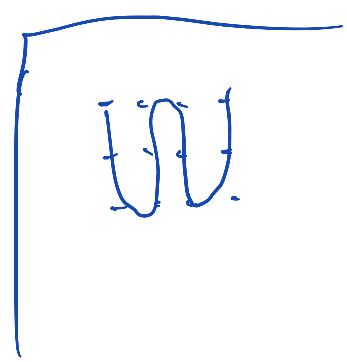
1D gapped: $D \sim 2^{\text{const}}$ (independent of system size)

1D critical: $D \sim 2^{\text{const} + c \ln L}$ ~ power law in L → efficient

2D gapped: $D \sim 2^{L}$

3D gapped: $D \sim 2^{L^2}$

} not efficient



Conclusion: MPS can encode ground state efficiently for gapped and gapless systems in 1D, but not 2D or 3D!

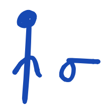
5. Tensor network diagrams

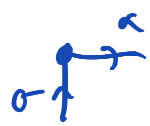
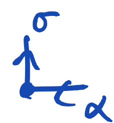
[Orus 2014, Sec 4.1]

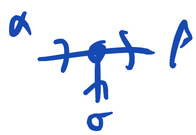
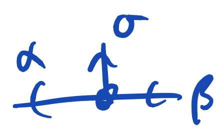
'tensor' = multi-dimensional array of numbers

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

rank-0: scalar A $\bullet$ $A^\dagger$ $\bullet$

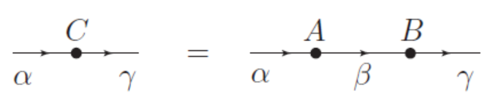
rank-1: vector $\underbrace{A^\sigma}_{\text{dual vectn}}$  $A^\dagger_\sigma$ 

rank-2: matrix $A^\sigma{}_\alpha$  $A^{\dagger\alpha}{}_\sigma$ 

rank-3: tensor $A^{\alpha\sigma}{}_\beta$  $A^{\dagger\beta}{}_{\cancel{\alpha\sigma}\,\sigma\alpha}$ 

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

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

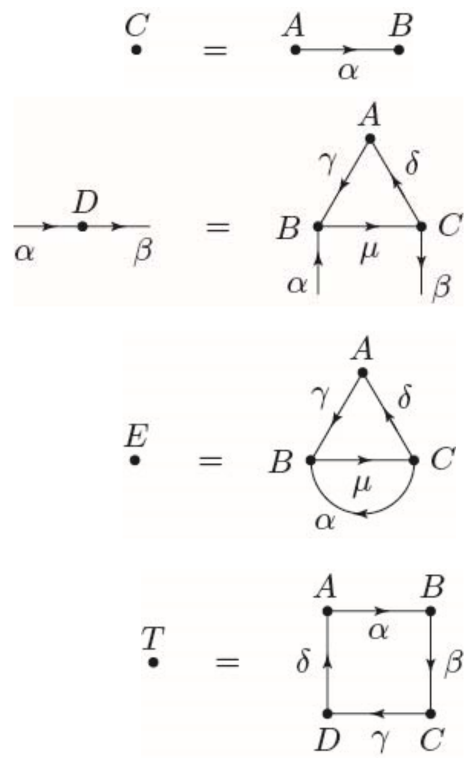
'tensor network' = set of tensors with some or all indices contracted according to some pattern

Examples:

Your try:

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

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

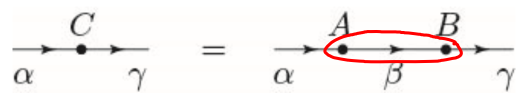


Answer:

Cost of computing contractions

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

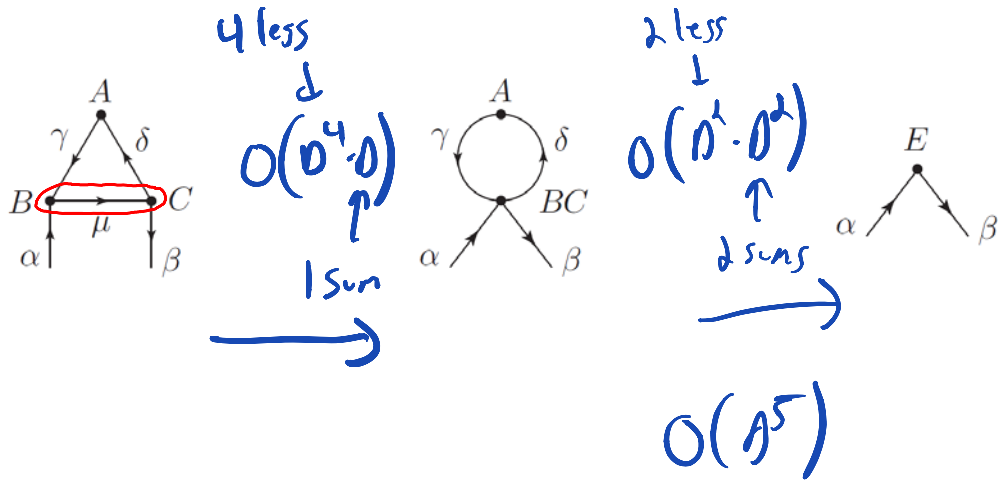
Example 1: cost of matrix multiplication is $O(D^3)$

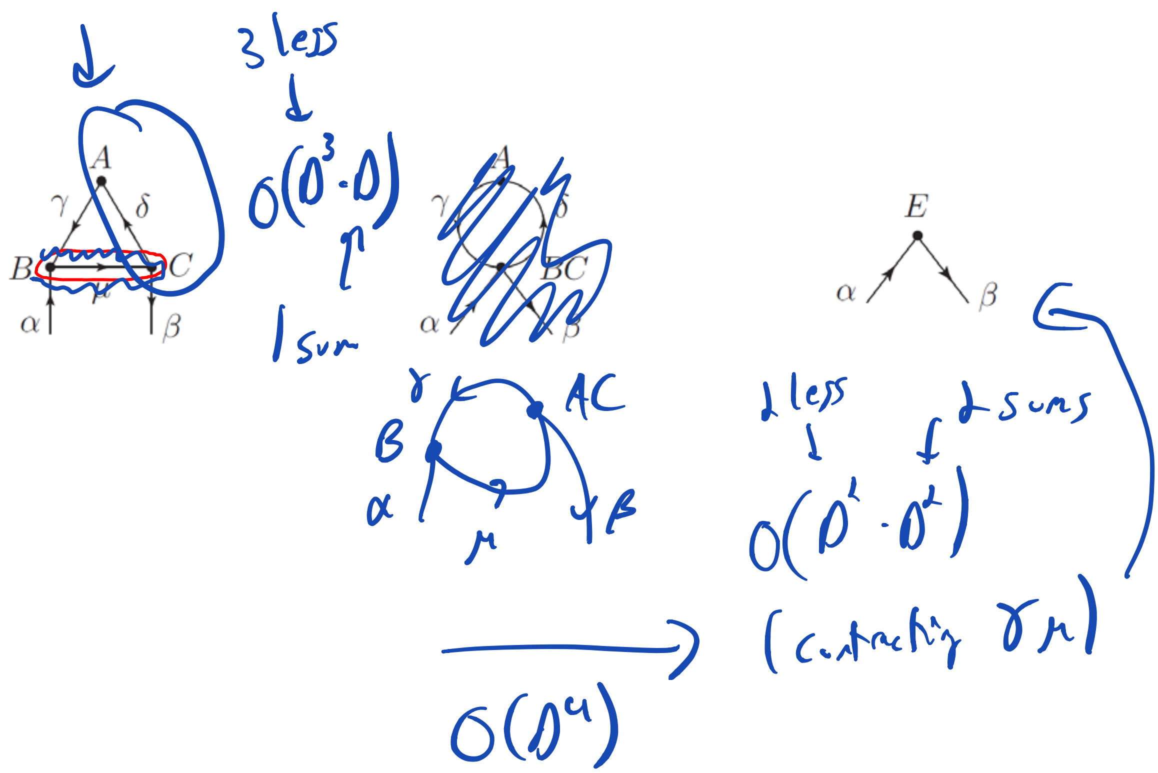


For every fixed α and γ ($D_\alpha \times D_\gamma$ combinations), sum over D_β values of β

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

Example 2:





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

Finding optimal contraction order is difficult. In practice, trial and error….

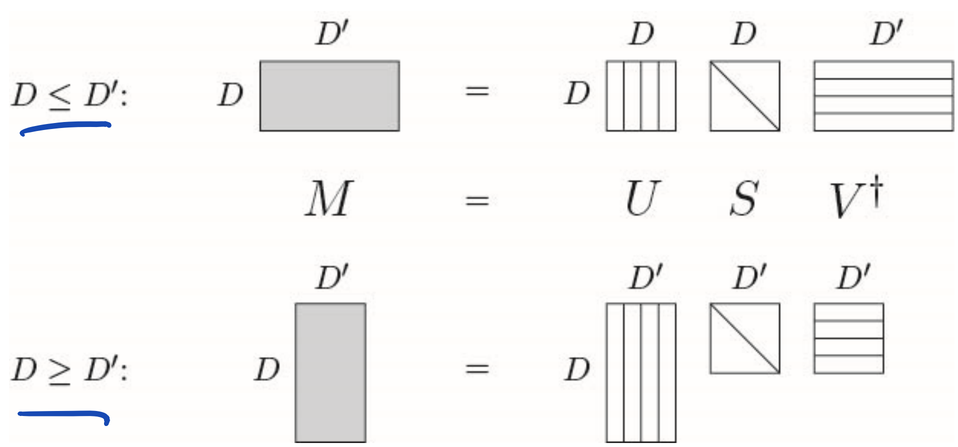
NP complete

In first part of course we will focus on 1D tensor networks, then 2D.

6. Singular value decomposition (SVD)

[Schollwoeck2011, Sec 4]

Any matrix M of dimension $D \times D'$ can be written as $M = USV^\dagger$

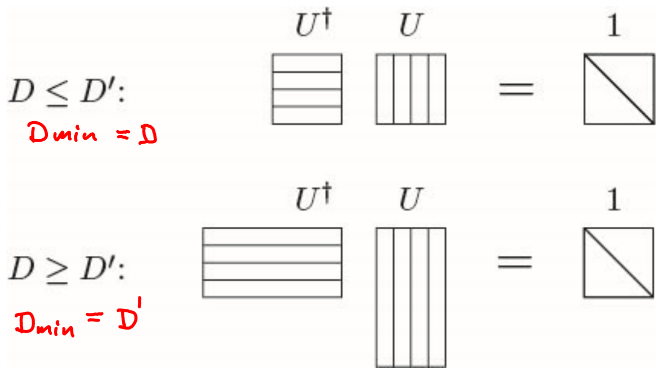


Properties of S

- square matrix of dimension $D_{min} \times D_{min}$ $\left(D_{min} = \min(D, D')\right)$
- diagonal with non-negative diagonal elements (singular values) $s_\alpha \equiv S_{\alpha\alpha}$
- Schmidt rank r : number of non-zero singular values
- arrange in descending order: $s_1 \geq s_2 \geq s_r > 0$

$$S = \mathrm{diag}(s_1, \dots, s_r, \underbrace{0 \dots 0}_{D_{min} - r})$$

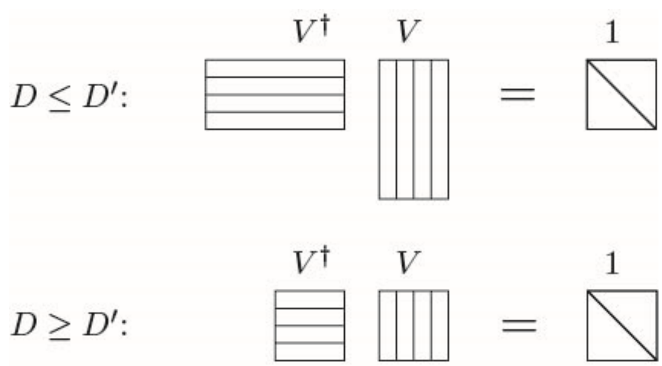
Properties of U:



- matrix of dimension
- columns are orthonormal

$$U^\dagger U = I$$

Properties of $V^\dagger$:



- matrix of dimension
- rows are orthonormal

$$V^\dagger V = I$$

Useful properties:

$$MM^\dagger = USV^\dagger \cdot VSU^\dagger = US^2U^\dagger$$

$$\Rightarrow \quad MM^\dagger U = US^2$$

$$M^\dagger M = VSU^\dagger USV^\dagger = VS^2V^\dagger$$

$$M^\dagger M V = VS^2$$

So columns of U are eigenvectors of $MM^\dagger$

Columns of V are eigenvectors of $M^\dagger M$

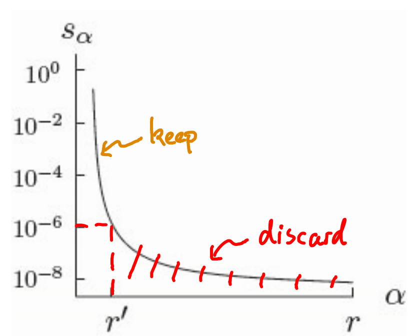
<u>Truncation</u>

SVD yields optimal approximation of rank r matrix M by a rank $r' < r$ matrix M'

(optimal wrt Frobenius norm:)

Suppose $M = USV^\dagger$

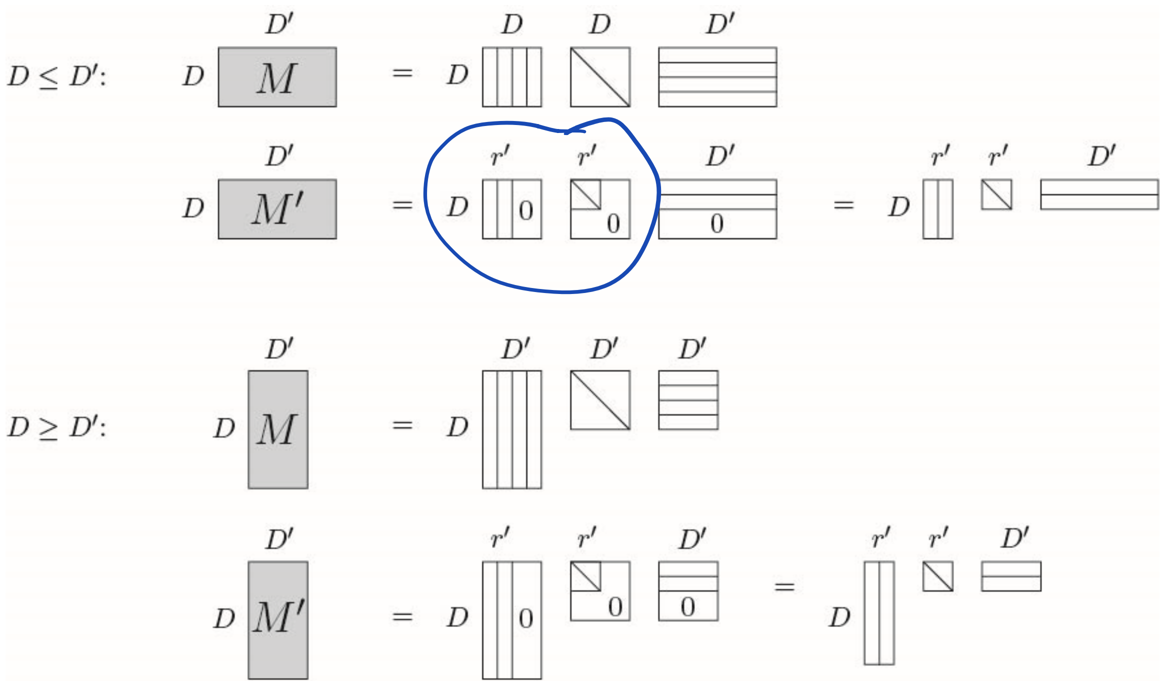
with



Truncate: $M' = US'V^\dagger$

with $S' = \text{diag}(s_1 \ldots s_{r'}, \underbrace{0 \ldots 0}_{D_{min} - r' \text{ zeros}})$

Retain only r' largest singular values! Visualization, with $r = D_{min}$:



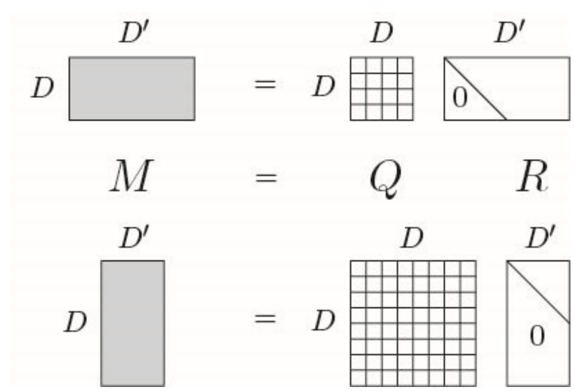
<u>QR decomposition</u>

If singular values are not needed,

a $D \times D'$ matrix M

has the 'full QR decomposition'

$M = QR$

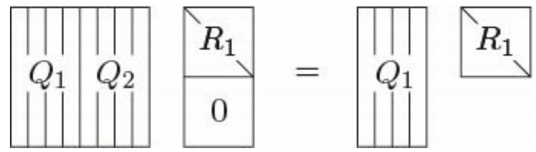


with Q a $D \times D$ unitary matrix $QQ^\dagger = Q^\dagger Q = I$

and R a $D \times D'$ upper triangular matrix $R_{\alpha\beta} = 0$ if $\alpha > \beta$.

If $D \geq D'$, then M has the 'thin QR decomposition'

$$M = (Q_1, Q_2) \cdot \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 \cdot R_1$$



rectangular

with dim(Q1) = $D \times D'$, dim(R1) = $D' \times D'$,

and R1 upper triangular.

$Q_1^\dagger Q_1 = I$ but $Q_1 Q_1^\dagger \neq I$

QR is numerically cheaper than SVD but has less information (does not provide rank).