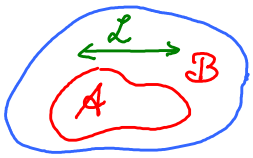
1. Entanglement Entropy and Area Laws (introductory comments)

Consider quantum system in 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 $\mathcal{L}$.

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

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

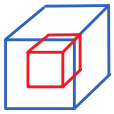
'Entanglement entropy' of $\mathcal{A}$ and $\mathcal{B}$: $S_{\mathcal{A}/\mathcal{B}} = -\mathrm{Tr}_{\mathcal{A}}\, \hat{\rho}_{\mathcal{A}} \log_2 \hat{\rho}_{\mathcal{A}} = -\sum_\alpha w_\alpha \log_2 w_\alpha$ (2)

(w_α: eigenvalues of $\hat{\rho}_{\mathcal{A}}$)

It turns out: for Hamiltonians with only local interactions, $S_{\mathcal{A}/\mathcal{B}}$ is governed by an 'area law':

$S \equiv S_{\mathcal{A}/\mathcal{B}} \sim$ (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)

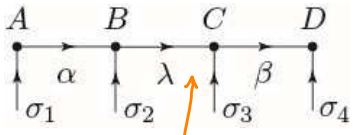
$\sim$ const. in 1D for gapped system (3c)

$\sim$ const. + $\ln N$ in 1D for gapless system (3d)

Now consider an MPS of maximal bond dimension D:

$|\psi\rangle = |\sigma_4\rangle \otimes |\sigma_3\rangle \otimes |\sigma_2\rangle \otimes |\sigma_1\rangle\, A^{\sigma_1}{}_{\alpha}\, B^{\alpha\sigma_2}{}_{\lambda}\, \mathbb{1}^{\lambda\bar{\lambda}}\, \mathbb{1}_{\bar{\lambda}\lambda'}\, C^{\lambda'\sigma_3}{}_{\beta}\, D^{\beta\sigma_4}$

unit tensor $\equiv \delta^{\lambda\bar{\lambda}}$; $\mathbb{1}_{\bar{\lambda}\lambda'} C^{\lambda'\sigma_3}{}_{\beta} \equiv C^{\sigma_3}{}_{\bar{\lambda}\beta}$

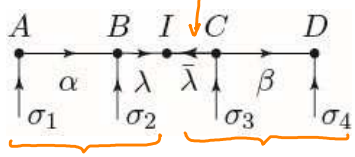


(4)

inserting $\mathbb{1} \cdot \mathbb{1}$ effectively inverts arrow

divide systems into two parts: Left: 2 sites, Right: 2 sites

system $\mathcal{A}$ system $\mathcal{B}$



$|\psi\rangle = \mathbb{1}^{\lambda\bar{\lambda}} \underbrace{|\sigma_4\rangle \otimes |\sigma_3\rangle\, C^{\sigma_3}{}_{\bar{\lambda}\beta}\, D^{\beta\sigma_4}}_{|\bar{\lambda}\rangle_R} \otimes \underbrace{|\sigma_2\rangle \otimes |\sigma_1\rangle\, A^{\sigma_1}{}_{\alpha}\, B^{\alpha\sigma_2}{}_{\lambda}}_{|\lambda\rangle_L}$

$= \sum_{\lambda\bar{\lambda}=1}^{D} \mathbb{1}^{\lambda\bar{\lambda}} |\bar{\lambda}\rangle_R \otimes |\lambda\rangle_L$ = entangled superposition of two state spaces, each having dimension of at most D (5)

$= \sum_{\lambda=1}^{D} |\lambda\rangle_R \otimes |\lambda\rangle_L$ (After the sum over $\bar{\lambda}$ has been performed explicitly using the Kronecker delta, the result contains non-covariantly paired indices.) (7)

suppress $\otimes$ henceforth

Density matrix: $\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{\lambda\lambda'} |\lambda\rangle_R |\lambda\rangle_L \, {}_L\langle\lambda'| \, {}_R\langle\lambda'|$ (8)

Reduced density matrix: $\hat{\rho}_A = \mathrm{Tr}_B \, \hat{\rho} = \sum_{\mu} {}_R\langle\mu| \sum_{\lambda\lambda'} |\lambda\rangle_R |\lambda\rangle_L \, {}_L\langle\lambda'| \, {}_R\langle\lambda'|\mu\rangle_R$ (9)

complete set of states for B

$= \sum_{\lambda\lambda'} |\lambda\rangle_L (\rho_A)^{\lambda}_{\lambda'} \, {}_L\langle\lambda'|$ (10)

with matrix elements

$(\rho_A)^{\lambda}_{\lambda'} = \sum_{\mu} {}_R\langle\mu|\lambda\rangle_R \, {}_R\langle\lambda'|\mu\rangle_R = \sum_{\mu} {}_R\langle\lambda'|\mu\rangle_R \, {}_R\langle\mu|\lambda\rangle_R = {}_R\langle\lambda'|\lambda\rangle_R$ (11)

$\sum_{\mu} |\mu\rangle\langle\mu| = \mathbb{1}_B$

This matrix has rank $\leq D$ (say $= D$) (rank = maximum number of linearly independent rows or column)

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

and normalization $1 = \mathrm{Tr} \, \hat{\rho}_A = \sum_{\alpha} w_\alpha$ (12)

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

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

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

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

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

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

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

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

2. Tensor network diagrams

[Orus 2014, Sec. 4.1]

TNB-II.2

'tensor' = multi-dimensional array of numbers

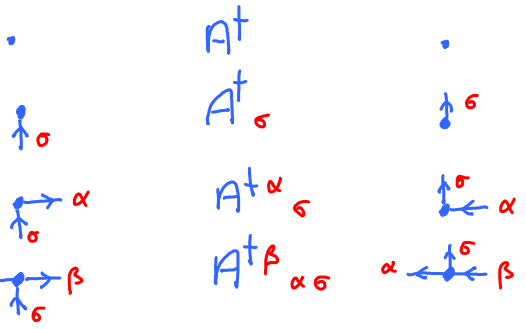
'rank of tensor' = number of indices = # of legs

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

rank-1: vector A^σ $A^\dagger_\sigma$

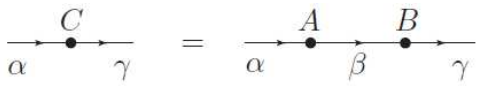
rank-2: matrix $A^\sigma{}_\alpha$ $A^{\dagger\alpha}{}_\sigma$

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



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; is often/usually not written explicitly)

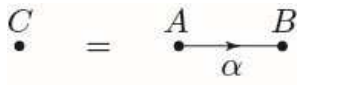
'open index' = non-contracted index (here α , γ)

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

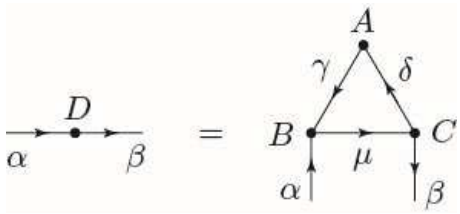
Examples:

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

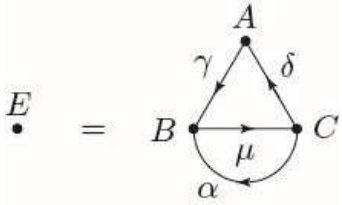
scalar vector · dual vector



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

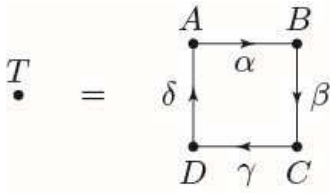


$$E = D^\alpha{}_\alpha = A^\delta{}_\gamma B^{\gamma\alpha}{}_\mu C^{\mu\delta}{}_\alpha$$



Trace of matrix product:

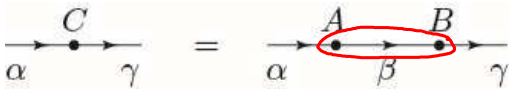
$$T = A^\delta{}_\alpha B^\alpha{}_\beta C^\beta{}_\gamma D^\gamma{}_\delta$$



Cost of computing contractions

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

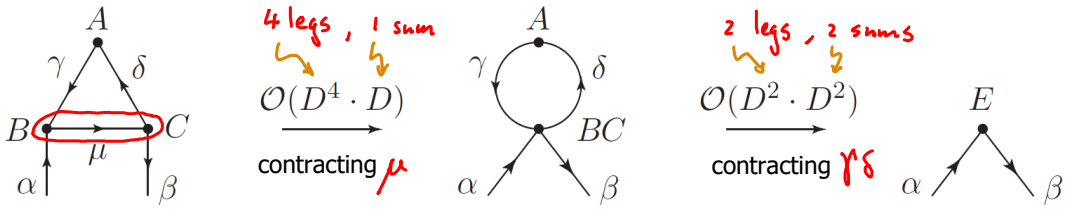
Example 1: cost of matrix multiplication is $\mathcal{O}(D^3)$:



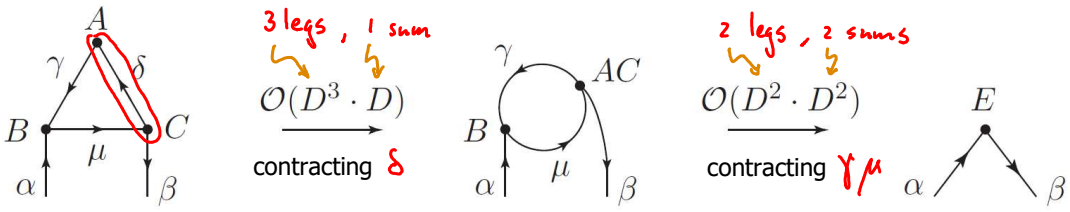
For every fixed α and γ ($D_\alpha \times D_\gamma$ combinations), sum over D_β values of β

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

Example 2:



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



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

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…

In first two-thirds of course, we will focus on 1D tensor networks. 2D will come after that.

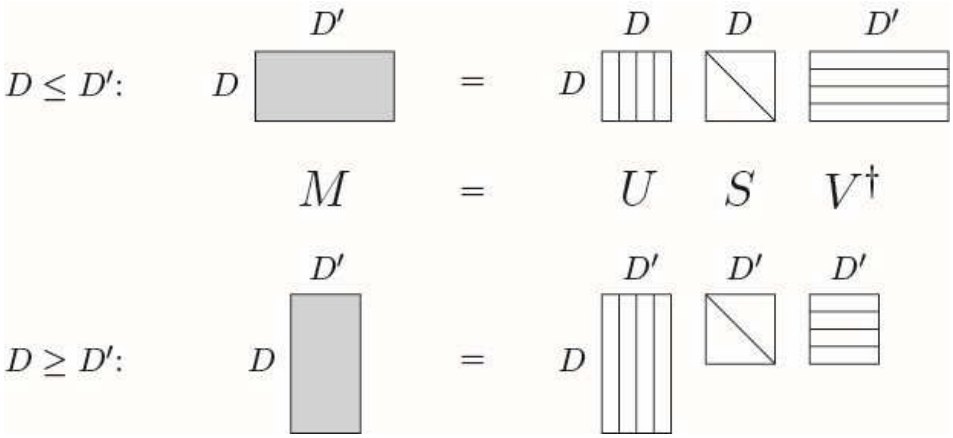
3. Singular value decomposition (SVD)

[Schollwoeck2011, Sec. 4]

TNB-II.3

Any matrix M of dimension $D \times D'$ can be written as

$$M = U S V^\dagger \qquad (1)$$



Properties of S

- square matrix, of dimension $D_{min} \times D_{min}$, with $D_{min} = \min(D, D')$
- diagonal, with non-negative diagonal elements, called 'singular values' $S_\alpha \equiv S_{\alpha\alpha}$

- 'Schmidt rank' r : number of non-zero singular values
- arrange in descending order: $S_1 \geq S_2 \geq \ldots \geq S_r > 0$

$$\Rightarrow \quad S = \mathrm{diag}(s_1, s_2, \ldots, s_r, \underbrace{0, \ldots, 0}_{D_{min} - r}) \qquad (2)$$

zeros

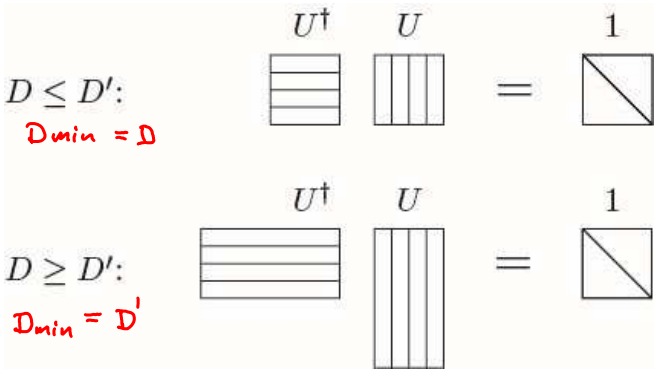
Properties of U :

- matrix of dimension $D \times D_{min}$
- columns are orthonormal:

$$U^\dagger U = \mathbb{1} \qquad (3)$$

but $U U^\dagger \neq \mathbb{1}$

(not unitary)



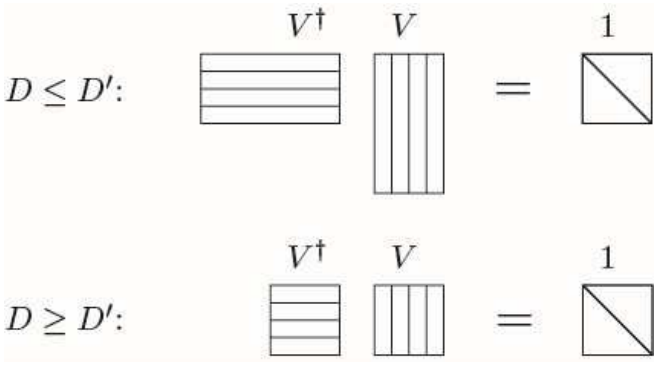
Properties of $V^\dagger$:

- matrix of dimension $D_{min} \times D'$
- rows are orthonormal:

$$V^\dagger V = \mathbb{1} \qquad (4)$$

but $V V^\dagger \neq \mathbb{1}$

(not unitary)



(1), (3), (4) imply:

$$MM^\dagger \overset{(1)}{=} USV^\dagger VSU^\dagger \overset{(4)}{=} US^2U^\dagger \overset{(3)}{\Rightarrow} MM^\dagger U = US^2 \qquad (5)$$

$$M^\dagger M \overset{(1)}{=} VSU^\dagger USV^\dagger \overset{(3)}{=} VS^2V^\dagger \overset{(4)}{\Rightarrow} M^\dagger MV = VS^2 \qquad (6)$$

So, columns of U are eigenvectors of $MM^\dagger$, and columns of V are eigenvectors of $M^\dagger M$.

Truncation

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

(optimal w.r.t. the Frobenius norm: $\|M\|_F^2 \equiv \sum_{\alpha\beta} |M_{\alpha\beta}|^2$)

Suppose $M = USV^\dagger$ (7)

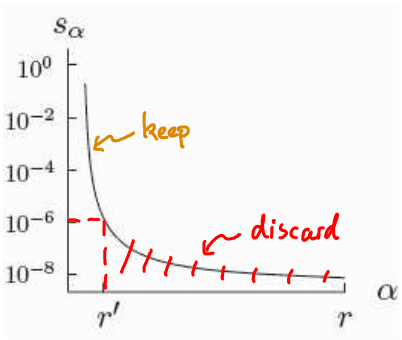
with $S = \mathrm{diag}(s_1, s_2, \ldots\ldots, s_r, 0, \ldots, 0)$ (8)

$D_{min} - r$ zeros

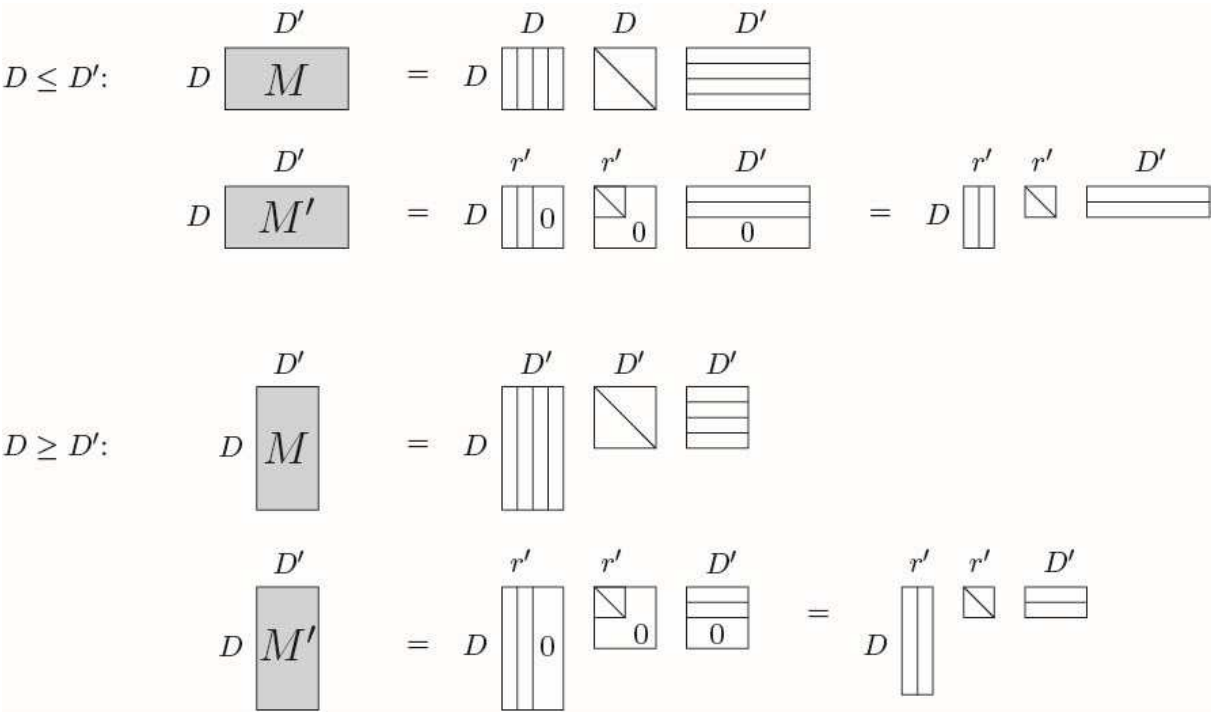
Truncate: $M' = US'V^\dagger$ (9)

with $S' = \mathrm{diag}(s_1, s_2, \ldots, s_{r'}, 0, \ldots, 0, \ldots, 0)$ (10)

$D_{min} - r'$ zeros



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



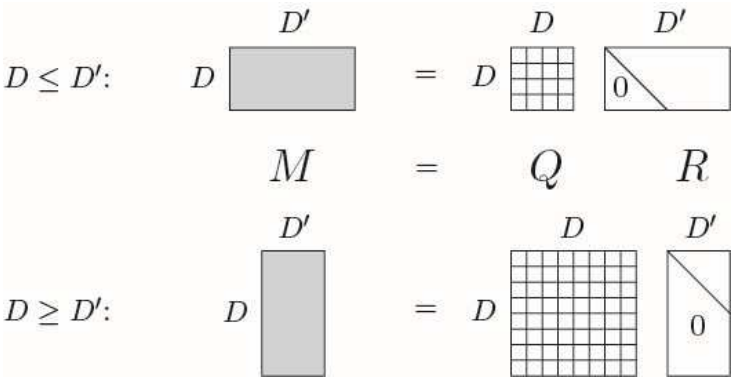
QR-decomposition

If singular values are not needed,

a $D \times D'$ matrix M

has the 'full QR decomposition'

$$M = Q R \qquad (11)$$

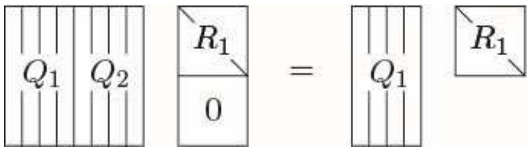


with Q a $D \times D$ unitary matrix, $Q Q^\dagger = Q^\dagger Q = \mathbb{1}$

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

If D ≥ D', then M has the 'thin QR decomposition'

$$M = (Q_1, Q_2) \cdot \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 \cdot R_1 \qquad (12)$$



with dim(Q1) = $D \times D'$, dim(R1) = $D' \times D'$, $Q_1^\dagger Q_1 = \mathbb{1}$ but $Q_1 Q_1^\dagger \neq \mathbb{1}$ (13)

and R1 upper triangular.

QR-decomposition is numerically cheaper than SVD, but has less information (not 'rank-revealing').