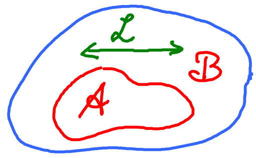
Tensor Network Basics II

TNB-II.1

1. Entanglement Entropy and Area Laws

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 $\mathcal{A}$):

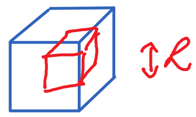
'reduced density matrix' for $\mathcal{A}$: $\hat\rho_{\mathcal{A}} \equiv \mathrm{Tr}_{\mathcal{B}}\,\hat\rho$ and $\hat\rho_{\mathcal{B}} \equiv \mathrm{Tr}_{\mathcal{A}}\,\hat\rho$ (1)

'Entanglement entropy' of $\mathcal{A}$ and $\mathcal{B}$: $S_{\mathcal{A}/\mathcal{B}} = -\mathrm{Tr}\,\hat\rho_{\mathcal{A}} \ln_2 \hat\rho_{\mathcal{A}} = -\sum_\alpha w_\alpha \ln_2 w_\alpha$ (2)

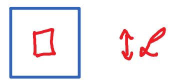
w_α: eigenvalues of $\hat\rho_{\mathcal{A}}$

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)



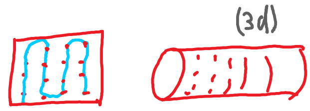
$\sim \mathcal{L}^2$ in 3D for gapped system (3a)



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

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

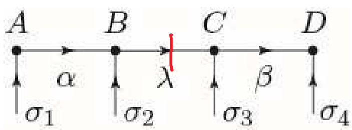
$\sim$ const. $+ \ln N$ in 1D for gapless system (3d)



Now consider an MPS of maximal bond dimension D:

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

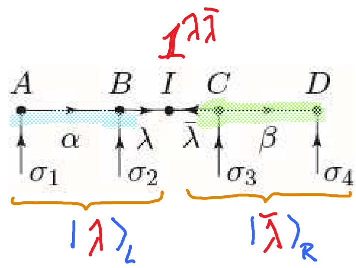
unit tensor $\equiv \delta^{\lambda\bar\lambda}$



(4)

divide systems into two parts: $\underbrace{\text{Left: 2 sites,}}_{\text{system}}$ $\underbrace{\text{Right: 2 sites}}_{\text{system}}$

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



$$= \sum_{\lambda\bar\lambda=1}^{D} \mathbb{1}^{\lambda\bar\lambda}\, |\bar\lambda\rangle_R \otimes |\lambda\rangle_L$$

= entangled superposition of two state spaces, each having dimension of at most D (5)

$$= \sum_{\lambda=1}^{D} |\lambda\rangle_R \otimes |\lambda\rangle_L$$

suppress $\otimes$ henceforth

(After the sum over $\bar\lambda$ has been performed explicitly using the Kronecker delta, the result contains non-covariantly paired indices.) (7)

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

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

complete set of states for B

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

with matrix elements

$$(\rho_A)^{\lambda}{}_{\lambda'} = \sum_{\mu} {}_R\langle\mu|\lambda\rangle_R \, {}_R\langle\lambda'|\mu\rangle_R = \sum_{\mu} \underbrace{{}_R\langle\lambda'|\mu\rangle_R \, {}_R\langle\mu|}_{\mathbb{1}_B}\lambda\rangle_R = {}_R\langle\lambda'|\lambda\rangle_R \qquad (11)$$

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

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

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

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 : $$\le - \sum_{\alpha=1}^{D} \frac{1}{D} \ln_2 \frac{1}{D} = \ln_2 D \qquad (13)$$

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

1D gapped: $D \overset{(3c)}{\sim} 2^{\text{const}}$ (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

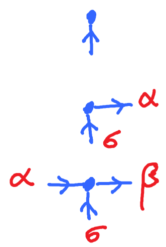
'rank of tensor' = number of indices = # of legs

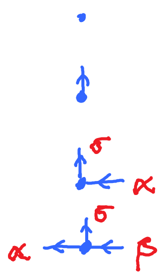
rank-0: scalar A $\qquad A^\dagger$

rank-1: vector A^σ $\qquad A^\dagger{}_\sigma$

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

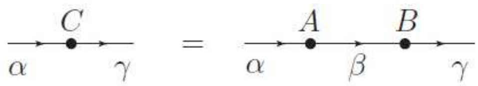
rank-3: tensor $A^{\alpha\sigma}{}_\beta$ $\qquad A^{\dagger\beta}{}_{\alpha\sigma}$





Index contraction: summation over repeated index

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



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)

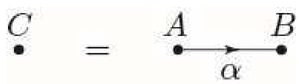
'open index' = non-contracted index (here α , β)

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

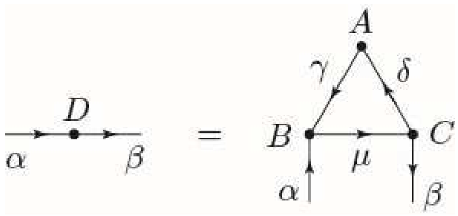
Examples:

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

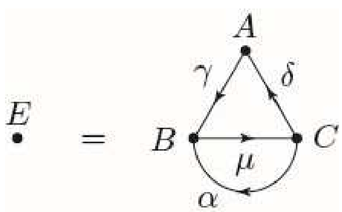
scalar $\qquad$ vector · dual vector



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

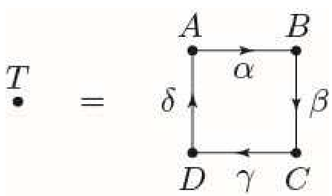


$$E = D^\alpha{}_\alpha = A^\delta{}_\gamma B^{\gamma\alpha}{}_\mu C^\mu{}_\alpha$$



Trace of matrix product:

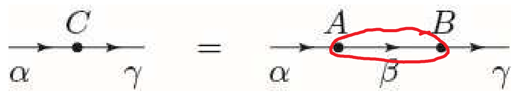
$$T = A^\delta{}_\alpha B^\alpha{}_\beta C^\beta{}_\gamma D^\gamma{}_\delta$$



Cost of computing contractions

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

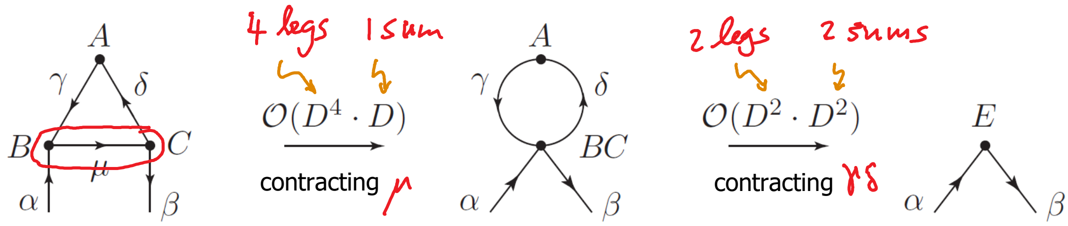
Example 1: cost of matrix multiplication is $\mathcal{O}(D^3)$:



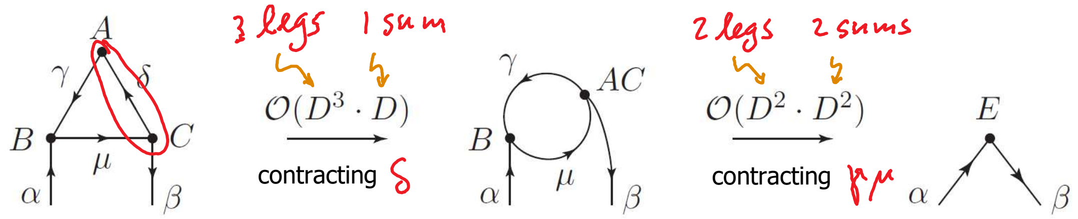
For every fixed α and γ ($D_\alpha \times D_\gamma$ combinations), sum over D_β values of β

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

Example 2:



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



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

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…

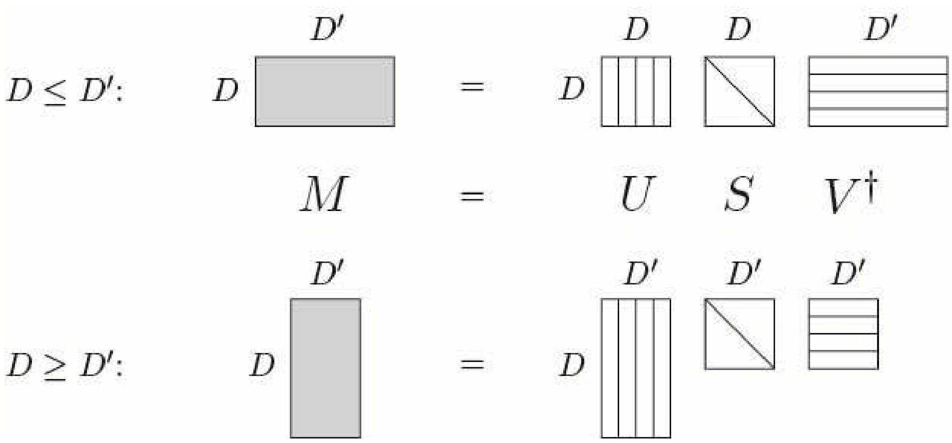
In first two-thirds of course, we will focus on 1D tensor networks. 2D will come after that.

3. Singular value decomposition (SVD)

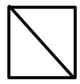
[Schollwoeck2011, Sec. 4]

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

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



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: $s_1 \ge s_2 \ge \dots \ge s_r > 0$

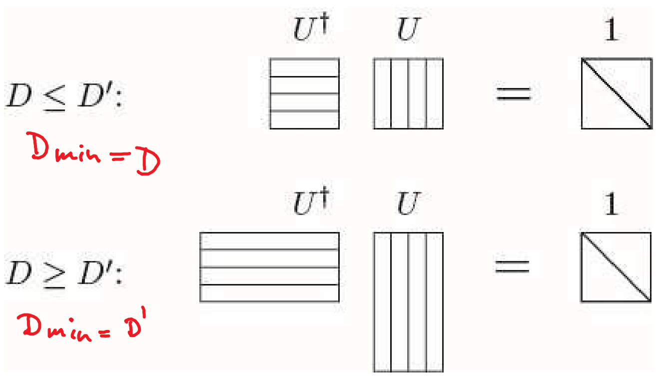
$$\Rightarrow \quad S = diag(s_1, s_2, \dots, s_r, \underbrace{0, \dots, 0}_{D_{min} - r \text{ zeros}}) \qquad (2)$$

Properties of U :

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

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

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

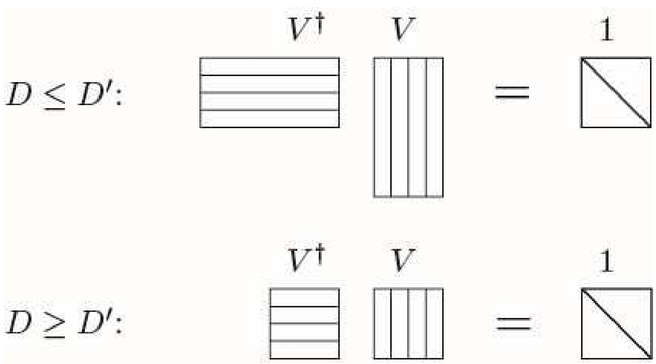


Properties of $V^\dagger$:

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

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

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



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

$$M M^\dagger \overset{(1)}{=} U S V^\dagger V S U^\dagger \overset{(4)}{=} U S^2 U^\dagger \overset{(3)}{\Rightarrow} U^\dagger M M^\dagger U = S^2 \qquad (5)$$

$$M^\dagger M \overset{(1)}{=} V S U^\dagger U S V^\dagger \overset{(3)}{=} V S^2 V^\dagger \overset{(4)}{\Rightarrow} V^\dagger M^\dagger M V = S^2 \qquad (6)$$

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' :

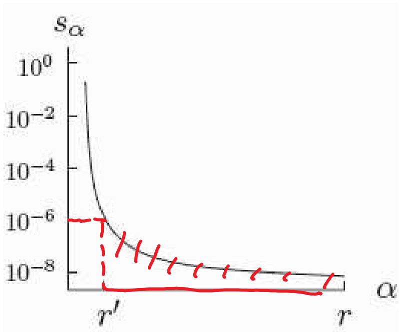
(optimal w.r.t. the Frobenius norm: $\|M\|_F^2 \equiv \sum_{\alpha\beta} |M_{\alpha\beta}|^2$)

Suppose $\quad M = U S V^\dagger \qquad (7)$

with $\quad S = \mathrm{diag}(s_1, s_2, \dots\dots, s_r, \underbrace{0, \dots, 0}_{D_{min} - r \text{ zeros}}) \qquad (8)$

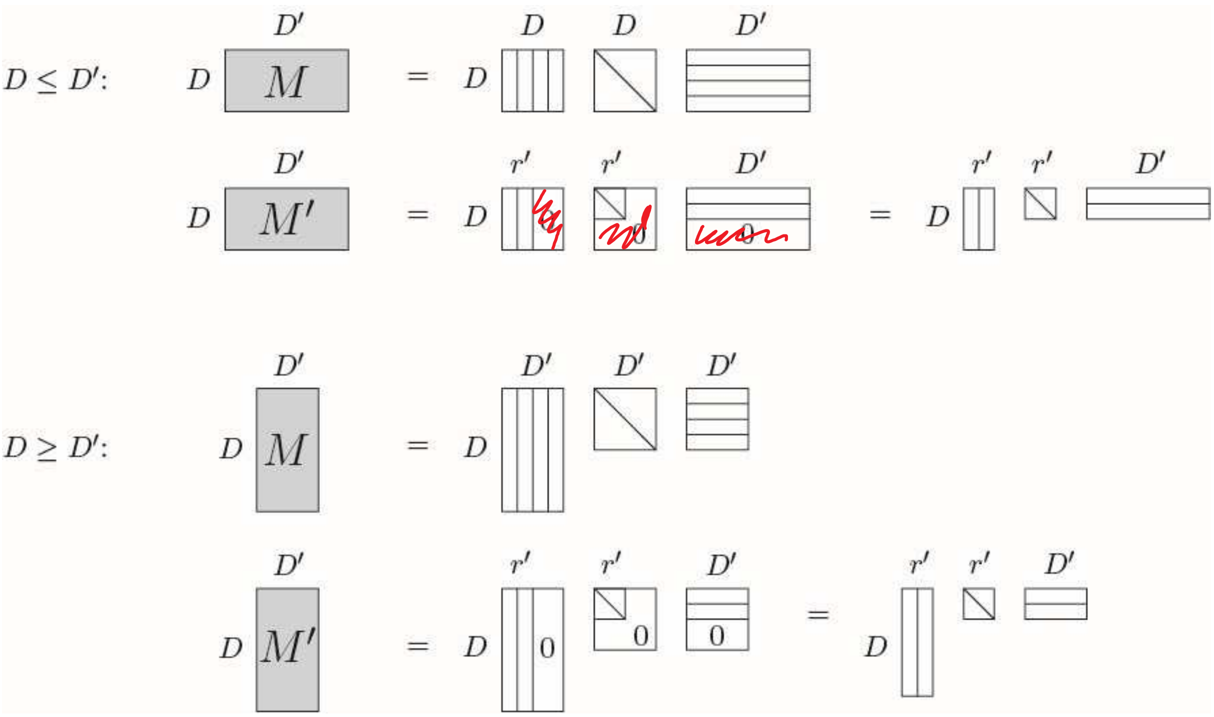
Truncate: $\quad \boxed{M' = U S' V^\dagger} \qquad (9)$

with $\quad S' = \mathrm{diag}(s_1, s_2, \dots, s_{r'}, \underbrace{\dots, 0, \dots, 0}_{D_{min} - r' \text{ zeros}}) \qquad (10)$



Retain only r' largest singular values!

Visualization, with $r = D_{min}$:

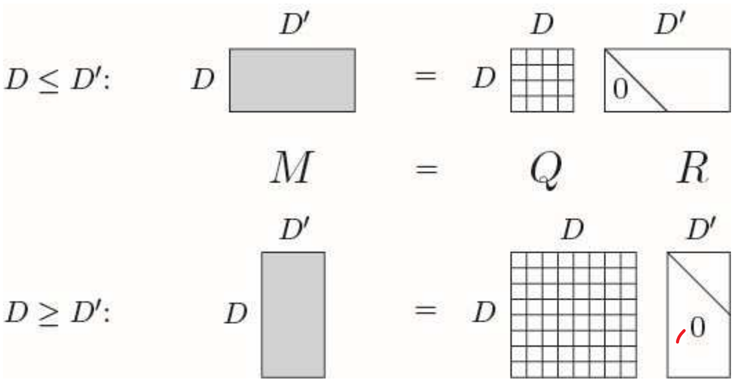


QR-decomposition

If singular values are not needed,

a $D \times D'$ matrix M

has the 'full QR decomposition'

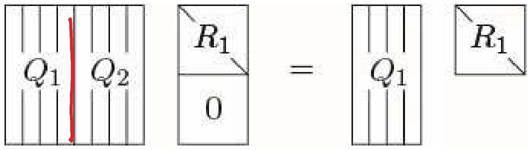


$$M = Q R \qquad (11)$$

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

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

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



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

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

and R1 upper triangular.

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