Tensor Network Basics III

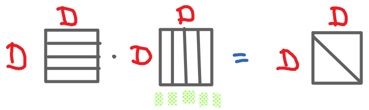
TNB-III.1

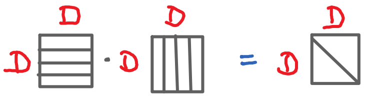
1. Unitaries and isometries (reminder)

Unitaries

A square matrix $\underset{D\times D}{U \in \mathrm{mat}(D, D; \mathbb{C})}$ is called 'unitary' if it satisfies:

$$U^\dagger U = \mathbb{1}_D \quad (1a) \quad \Leftrightarrow \quad U U^\dagger = \mathbb{1}_D \quad (1b)$$



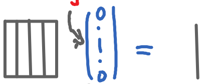


Its column vectors, $U = (\vec{u}_1, \vec{u}_2, \dots, \vec{u}_D)$, form a basis for $\mathbb{C}^D$ (2)

Its D row vectors also form a basis for $\mathbb{C}^D$

position j column j

U defines an invertible map:



$= \vec{u}_j \in \mathbb{C}^D, \quad j = 1, \dots, D$ (3a)

standard basis vector in $\mathbb{C}^D$

$$U : \mathbb{C}^D \to \mathbb{C}^D, \quad \vec{e}_j \mapsto U\vec{e}_j := \vec{e}_i U^i{}_j = \vec{u}_j \quad (i, j \in 1, \dots D) \quad (3b)$$

standard basis vector in $\mathbb{C}^D$: $\vec{e}_i = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ ← position i

Its inverse is given by

$$U^{-1} = U^\dagger : \mathbb{C}^D \to \mathbb{C}^D, \quad \vec{e}_i \longmapsto U^\dagger(\vec{e}_i) = \vec{e}_k U^{\dagger k}{}_i \quad (4)$$

Indeed, then $U^\dagger \vec{u}_j \overset{(3b)}{=} U^\dagger \vec{e}_i U^i{}_j \overset{(4)}{=} \vec{e}_k \underbrace{U^{\dagger k}{}_i U^i{}_j}_{(1a) = \delta^k{}_j} = \vec{e}_j$ ✓ (5)

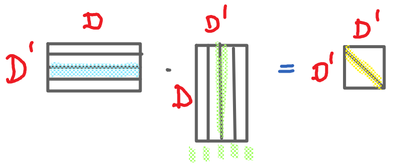
consistent with (3b)

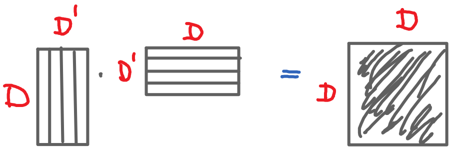
Left isometry

(isometry = distance-preserving map)

A rectangular matrix $A \in \mathrm{mat}(D, D'; \mathbb{C})$ with $D > D'$ is called a 'left isometry' if it satisfies:

$$A^\dagger A = \mathbb{1} \quad (6a) \qquad \text{Then} \quad A A^\dagger \neq \mathbb{1} \quad (6b)$$





Its D' column vectors, $A = (\vec{a}_1, \vec{a}_2, \dots, \vec{a}_{D'})$, are orthonormal, $\vec{a}_i^\dagger \cdot \vec{a}_j \overset{(6a)}{=} \delta_{ij}$. (7)

They form a basis for a D'-dimensional subspace of $\mathbb{C}^D$ $\quad \vec{a}_i^\dagger = \bar{\vec{a}}_i^{\,T}$

They form a basis for a D'-dimensional subspace of $\mathbb{C}^D$, $\qquad \vec{a}_i^{\dagger} = \bar{\vec{a}}_i^{T}$

space of D-dimensional colunmn vectors (8)

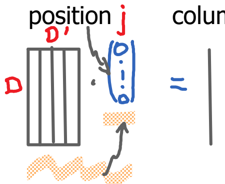
say $V_A = \mathrm{span}\{\vec{a}_1, \vec{a}_2, \dots, \vec{a}_{D'}\} \subsetneq \mathbb{C}^D$

subpace

[The D row vectors of A each are elements of $\mathbb{C}^{*D'}$, <u>not</u> $\mathbb{C}^{*D}$]

dual space of D'-dimensional row vectors

A defines an isometric map:



$$= \vec{a}_j \in \mathbb{C}^D, \qquad j = 1, \dots, D' \qquad (9a)$$

standard basis vector in $\mathbb{C}^{D'}$

Formally:

$$A : \mathbb{C}^{D'} \to \mathbb{C}^D, \qquad \vec{f}_j \mapsto A\vec{f}_j := \vec{e}_i A^i{}_j = \vec{a}_j \qquad j \in 1, \dots, D' \quad i \in 1, \dots, D \qquad (9b)$$

short column vectors $\qquad$ long column vectors

standard basis vector in $\mathbb{C}^D$

(9b): many (D) long columns are superposed to yield a smaller number (D') of orthonormal long columns.

These span $V_A \subsetneq \mathbb{C}^D$, the 'image space of A ' or 'image of ', with dimension $\dim(A) = D'$.

because A has fewer columns than rows

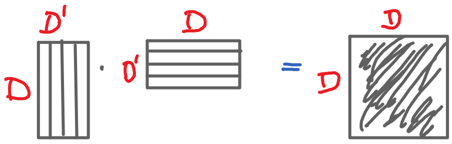
<u>Invariance of scalar product</u> (hence the name: iso-metric = equal metric):

If $A : \mathbb{C}^{D'} \to \mathbb{C}^D$, $\vec{x} \mapsto \vec{y} = A\vec{x}$, then

$$\|\vec{y}\|^2_D = \vec{y}^{\dagger} \cdot \vec{y} = \vec{x}^{\dagger} \underbrace{A^{\dagger} A}_{\mathbb{1}_{D'}} \vec{x} = \vec{x}^{\dagger} \cdot \vec{x} = \|\vec{x}\|^2_{D'} \qquad (10)$$

<u>Left projector</u>

$$= P = A A^{\dagger} =$$



(11)

is a projector, since $P^2 = (A \underbrace{A^{\dagger})(A}_{\mathbb{1}_{D'}} A^{\dagger}) = A A^{\dagger} = P$ (12)

(6a)

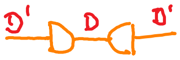
Its action leaves V_A invariant, because it leaves each its basis vectors invariant: (13)

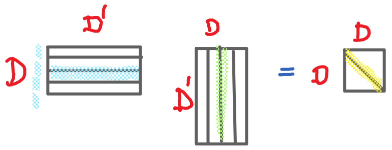
$$P\vec{a}_j \overset{(11,9b)}{=} A \underbrace{A^{\dagger} A}_{(6a) = \mathbb{1}} \vec{f}_j = A \vec{f}_j \overset{(9b)}{=} \vec{a}_j$$

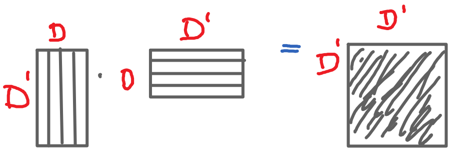
Right isometry

A rectangular matrix $B \in \mathrm{mat}(D, D'; \mathbb{C})$ with $D < D'$ is called a 'right isometry' if it satisfies:

$$B B^\dagger = \mathbb{1}_D \qquad (14a) \qquad \text{Then} \quad B^\dagger B \neq \mathbb{1}_{D'} \qquad (14b)$$







Its D row vectors, $B = \begin{pmatrix} \vec b^1 \\ \vec b^2 \\ \vdots \\ \vec b^D \end{pmatrix}$, are orthonormal, $\vec b^i \cdot \vec b^{\dagger}{}_j \overset{(6a)}{=} \delta^i{}_j$. (15)

[row vectors (dual to column vectors) are labeled using upstairs index]

They form a basis for a D-dimensional subspace of $\mathbb{C}^{*D'}$, ← space of D'-dimensional row vectors

say $V_B^* = \mathrm{span}\{\vec b^1, \vec b^2, \ldots, \vec b^D\} \subsetneq \mathbb{C}^{*D'}$ (16)

subpace

[The D' column vectors of B each are elements of $\mathbb{C}^D$, <u>not</u> $\mathbb{C}^{D'}$.]

B defines an isometric map: $(0.. 1..0) \cdot$

$= \vec b^i \in \mathbb{C}^{*D}, \quad i = 1, \ldots, D'$ (17a)

position i

standard basis vector in $\mathbb{C}^{*D'}$

$B : \mathbb{C}^{*D'} \to \mathbb{C}^{*D}$, $\vec f^i \mapsto \vec f^i B := B^i{}_j \, \vec e^j = \vec b^i$ $\quad i \in 1, \ldots, D'$, $j \in 1, \ldots, D$ (17b)

short row vectors — long row vectors

standard basis vector in $\mathbb{C}^{*D}$

(17b) says: many (D) long rows are superposed to yield a smaller number (D') of orthonormal long rows.

These span $V_B^* \subsetneq \mathbb{C}^{*D}$, the 'image space of B' or 'image of B', with dimension $\dim(B) = D'$.

because B has fewer rows than columns

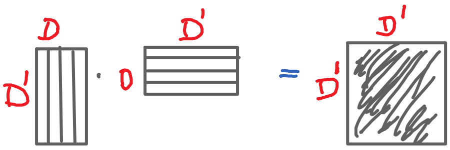
<u>Invariance of scalar product</u> (hence the name: iso-metric = equal metric):

If $B : \mathbb{C}^{*D'} \to \mathbb{C}^{*D}$, $\vec x \mapsto \vec y = \vec x B$, then

$$\|\vec y\|^2_{*D} = \vec y \cdot \vec y^\dagger = x \underbrace{B B^\dagger}_{\mathbb{1}_{D'}} x^\dagger = \vec x \cdot \vec x^\dagger = \|\vec x\|^2_{*D'} \qquad (18)$$

Right projector

$$= P = B^\dagger B =$$



(19)

is a projector, since $$P^2 = (B^\dagger \underbrace{B)(B^\dagger}_{\mathbb{1}_D} B) = B^\dagger B = P$$ (20)

(14a)

Its action leaves V_B^* invariant, since it leaves its basis vectors invariant:

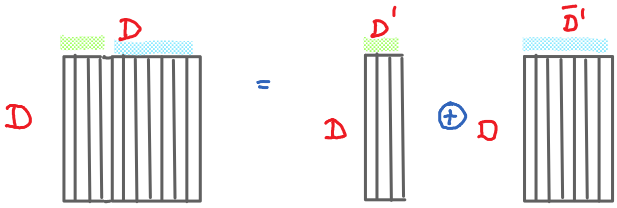
$$\vec{b}^i P \overset{(19,17b)}{=} \vec{f}^i \underbrace{B B^\dagger}_{(14a) = \mathbb{1}} B = \vec{f}^i B \overset{(17b)}{=} \vec{b}^i \quad ✓$$ (21)

Truncation of unitaries yield isometries

Consider a unitary, $D \times D$ matrix, $$U^\dagger U = \mathbb{1}_D \, ,$$ (22)

and partition its columns into two groups, containing D' and $\bar{D}' = D - D'$ columns:

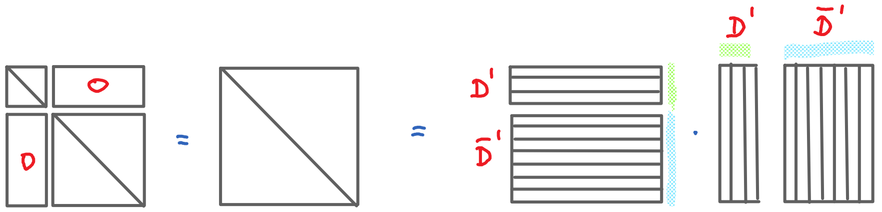
$$U = (\vec{u}_1, \vec{u}_2, \dots \vec{u}_{D'}, \vec{u}_{D'+1}, \dots \vec{u}_D) = (\vec{u}_1, \dots, \vec{u}_{D'}) \oplus (\vec{u}_{D'+1}, \dots, \vec{u}_D) =: A \oplus \bar{A}$$ (23)



(24)

Unitarity of U implies:

$$\begin{pmatrix} \mathbb{1}_{D'} & \\ & \mathbb{1}_{\bar{D}'} \end{pmatrix} = \mathbb{1}_D = U^\dagger U = \begin{pmatrix} A^\dagger \\ \bar{A}^\dagger \end{pmatrix} (A \, , \, \bar{A}) = \begin{pmatrix} A^\dagger A & A^\dagger \bar{A} \\ \bar{A}^\dagger A & \bar{A}^\dagger \bar{A} \end{pmatrix}$$ (25)

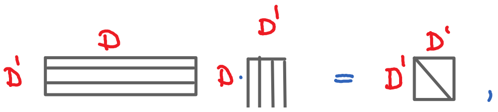


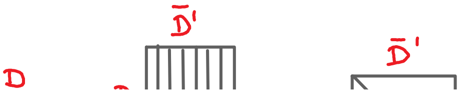
(26)

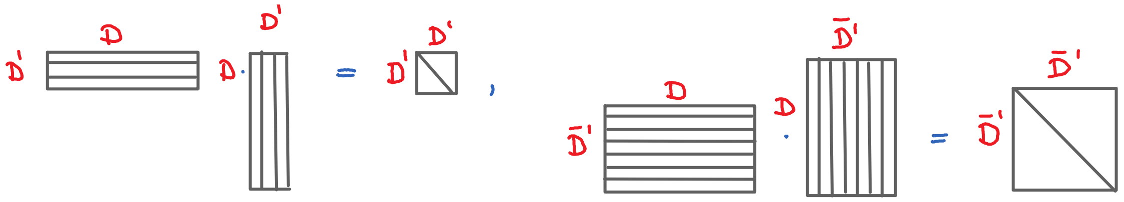
Hence, A and $\bar{A}$ are both isometries:

$$= A^\dagger A \overset{(25)}{=} \mathbb{1}_{D'} \, ,$$

$$= \bar{A}^\dagger \bar{A} \overset{(25)}{=} \mathbb{1}_{\bar{D}'}$$ (27)

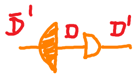






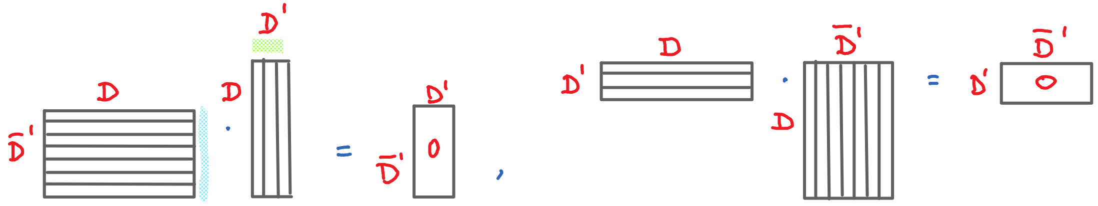
(28)

Moreover, A are $\bar{A}$ orthogonal to each other, since they are built from orthogonal column vectors:



$= \bar{A}^\dagger A \overset{(25)}{=} 0$,

$= A^\dagger \bar{A} \overset{(25)}{=} 0$ (29)



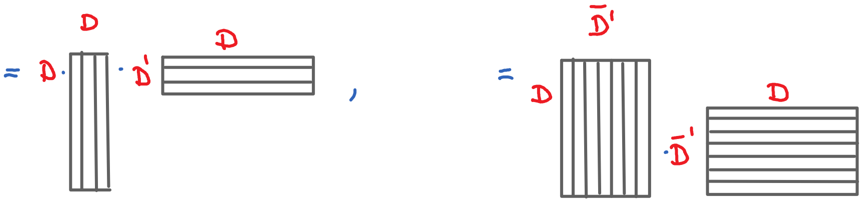
(30)

Complementary projectors

The projectors, $P = AA^\dagger =$

, $\bar{P} = \bar{A}\bar{A}^\dagger =$

(31)

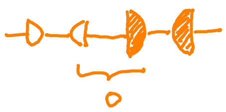


are both $D \times D$ matrices,

and satisfy orthonormality relations: (32)

$$P\cdot P \overset{(27)}{=} P \ , \quad \bar{P}\cdot\bar{P} \overset{(27)}{=} \bar{P} \ , \quad P\cdot\bar{P} \overset{(29)}{=} 0 \ , \quad \bar{P}\cdot P \overset{(29)}{=} 0 \qquad (33)$$

E.g.: $P\cdot\bar{P} = A \underbrace{A^\dagger \bar{A}}_{(29)\ =\ 0} \bar{A}^\dagger =$



$= 0$ (34)

They split $\mathbb{C}^D$ into two orthogonal and hence complementary subspaces:

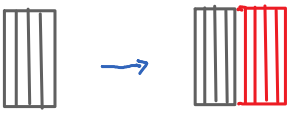
$$P : \mathbb{C}^D \to \mathbb{V}_A = \mathrm{span}\{\vec{u}_1, \dots \vec{u}_{D'}\} =: \mathrm{span}\{\vec{a}_1, \dots, \vec{a}_{D'}\} \subsetneq \mathbb{C}^D \qquad (35)$$

$$\bar{P} : \mathbb{C}^D \to \mathbb{V}_{\bar{A}} = \mathrm{span}\{\vec{u}_{D'+1}, \dots, \vec{u}_D\} =: \mathrm{span}\{\vec{\bar{a}}_1, \dots, \vec{\bar{a}}_{\bar{D}'}\} \subsetneq \mathbb{C}^D \qquad (36)$$

with $\vec{x}^\dagger \cdot \vec{y} = 0 \quad \forall \ \vec{x} \in \mathbb{V}_A , \ \vec{y} = \mathbb{V}_{\bar{A}}$ (37)

In this sense, isometries (more precisely, their projectors) map large vector spaces into smaller ones.

Conversely: any left (or right) isometry can be extended to a unitary by adding orthonormal columns (or rows) orthogonal to those already present.



(38)

(39)

2. Singular value decomposition (SVD)

[Schollwoeck2011, Sec. 4]

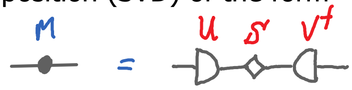
TNB-III.2

ttps://en.wikipedia.org/wiki/Singular_value_decomposition

Consider a $D \times D'$ matrix, $M \in \mathrm{mat}(D, D'; \mathbb{C})$ and let $\tilde{D} = \min(D, D')$ (1)

Theorem: (without proof) Any such M has a singular value decomposition (SVD) of the form

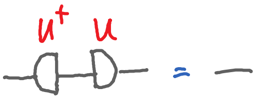
$$\boxed{\underset{D\times D'}{M} = \underset{D\times\tilde{D}}{U} \cdot \underset{\tilde{D}\times\tilde{D}}{S} \cdot \underset{\tilde{D}\times D'}{V^\dagger}}$$



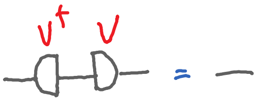
(2)

where

$U \in \mathrm{mat}(D, \tilde{D}; \mathbb{C})$ satisfies $\boxed{U^\dagger U = \mathbb{1}_{\tilde{D}}}$ (3)



$V^\dagger \in \mathrm{mat}(\tilde{D}, D'; \mathbb{C})$ satisfies $\boxed{V^\dagger V = \mathbb{1}_{\tilde{D}}}$ (4)



$S \in \mathrm{mat}(\tilde{D}, \tilde{D}; \mathbb{C})$ is diagonal, with purely non-negative diagonal elements. (5)

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Remarks:

(i) SVD ingredients can be found by diagonalization of the hermitian matrices $MM^\dagger$ and $M^\dagger M$.

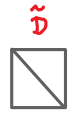
$$D\times D: \quad MM^\dagger \overset{(2)}{=} (US\underbrace{V^\dagger)(V}_{\mathbb{1}}SU^\dagger) \overset{(4)}{=} US^2U^\dagger \overset{(3)}{\Rightarrow} D\times\tilde{D}: \quad MM^\dagger U = US^2 \qquad (6)$$

$$D'\times D': \quad M^\dagger M \overset{(2)}{=} (VS\underbrace{U^\dagger)(U}_{}SV^\dagger) \overset{(3)}{=} VS^2V^\dagger \overset{(4)}{\Rightarrow} D'\times\tilde{D}: \quad M^\dagger MV = VS^2 \qquad (7)$$

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

(ii) Properties of S

- diagonal matrix, of dimension $\tilde{D} \times \tilde{D}$, with $\tilde{D} = \min(D, D')$ (8)
- diagonal elements can be chosen non-negative, are called 'singular values' $S_\alpha := S_{\alpha\alpha} =$ $\tilde{D}$



- 'Schmidt rank' r : number of non-zero singular values
- arrange in descending order: $s_1 \geq s_2 \geq \ldots \geq s_r > 0$ (9)

$$\Rightarrow \quad S = \mathrm{diag}(s_1, s_2, \ldots, s_r, \underbrace{0, \ldots, 0}_{\tilde{D}-r}) \qquad (10)$$

zeros

(iii) Properties of U and $V^\dagger$: $\tilde{D} = \min(D, D')$

- $\dim(U) = D \times \tilde{D}$, $\boxed{U^\dagger U = \mathbb{1}}$, columns of U are orthonormal. (11)

- $\dim(U) = D \times \tilde{D}$, $\boxed{U^\dagger U = \mathbb{1}_{\tilde{D}}}$, columns of U are orthonormal. (11)

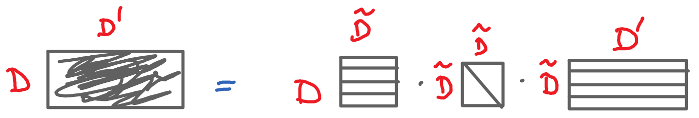
- If $D = \tilde{D}$, then U is unitary. If $D > \tilde{D}$, then U is a left isometry. (12)

- $\dim(V^\dagger) = \tilde{D} \times D'$, $\boxed{V^\dagger V = \mathbb{1}_{\tilde{D}}}$, rows $V^\dagger$ of are orthonormal. (13)

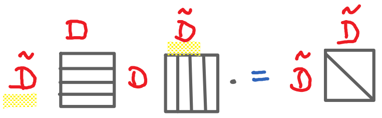
- If $\tilde{D} = D'$, then $V^\dagger$ is unitary. If $\tilde{D} < D'$, then $V^\dagger$ is a right isometry. (14)

(iv) Visualization

If $\tilde{D} = D \leq D'$:

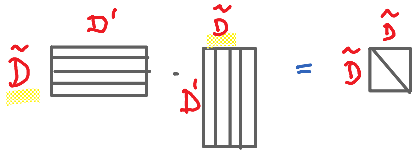
$M =$ 

$= U \cdot S \cdot V^\dagger$ (15)

U is unitary: $U^\dagger U =$ 

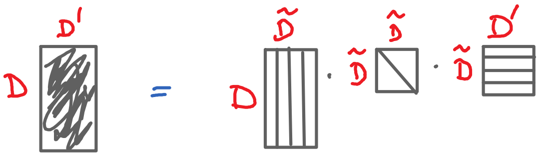
$= \mathbb{1}_{\tilde{D}}$ (16)

product is arranged such that the outer indices have the smallest dimension, $\tilde{D}$

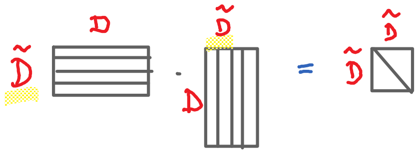
$V^\dagger$ is right isometry: $V^\dagger V =$ 

$= \mathbb{1}_{\tilde{D}}$ (17)

If $D \geq D' = \tilde{D}$:

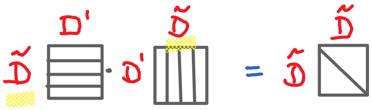
$M =$ 

$= U \cdot S \cdot V^\dagger$ (18)

U is left isometry: $U^\dagger U =$ 

$= \mathbb{1}_{\tilde{D}}$ (19)

product is arranged such that the outer indices have the smallest dimension, $\tilde{D}$

$V^\dagger$ is unitary: $V^\dagger V =$ 

$= \mathbb{1}_{\tilde{D}}$ (20)

Truncation via SVD

Def: Frobenius norm: $\|M\|_F^2 := \sum_{\alpha\beta} |M_{\alpha\beta}|^2 = \sum_{\alpha\beta} \overline{M_{\alpha\beta}}\, M_{\alpha\beta} = \sum_{\alpha\beta} \underline{M^\dagger_{\beta\alpha} M_{\alpha\beta}} = \mathrm{Tr}\, M^\dagger M$ (21)

Def: Frobenius norm: $\|M\|_F := \sum_{\alpha\beta} |M_{\alpha\beta}|^2 = \sum_{\alpha\beta} M_{\alpha\beta} M_{\alpha\beta} = \sum_{\alpha\beta} M^T_{\beta\alpha} M_{\alpha\beta} = \mathrm{Tr}\, M^\dagger M$ (21)

evaluated via SVD: $= \mathrm{Tr}\,(V S \underbrace{U^\dagger U}_{=1} S V^\dagger) = \mathrm{Tr}\,(\underbrace{V^\dagger V}_{=1} S^2) = \boxed{\mathrm{Tr}\, S^2}$ (22)

trace is cyclic

singular values determine norm

Truncation

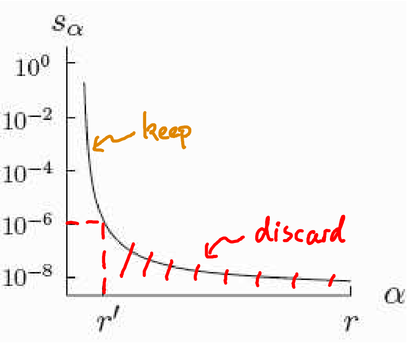
SVD can be used to approximate a rank r matrix M by a rank $r'\ (<r)$ matrix M' :

Suppose $M = U S V^\dagger$ (23)

with $S = \mathrm{diag}(s_1, s_2, \ldots\ldots\ldots, s_r, \underbrace{0, \ldots, 0}_{\tilde D - r \text{ zeros}})$ (24)

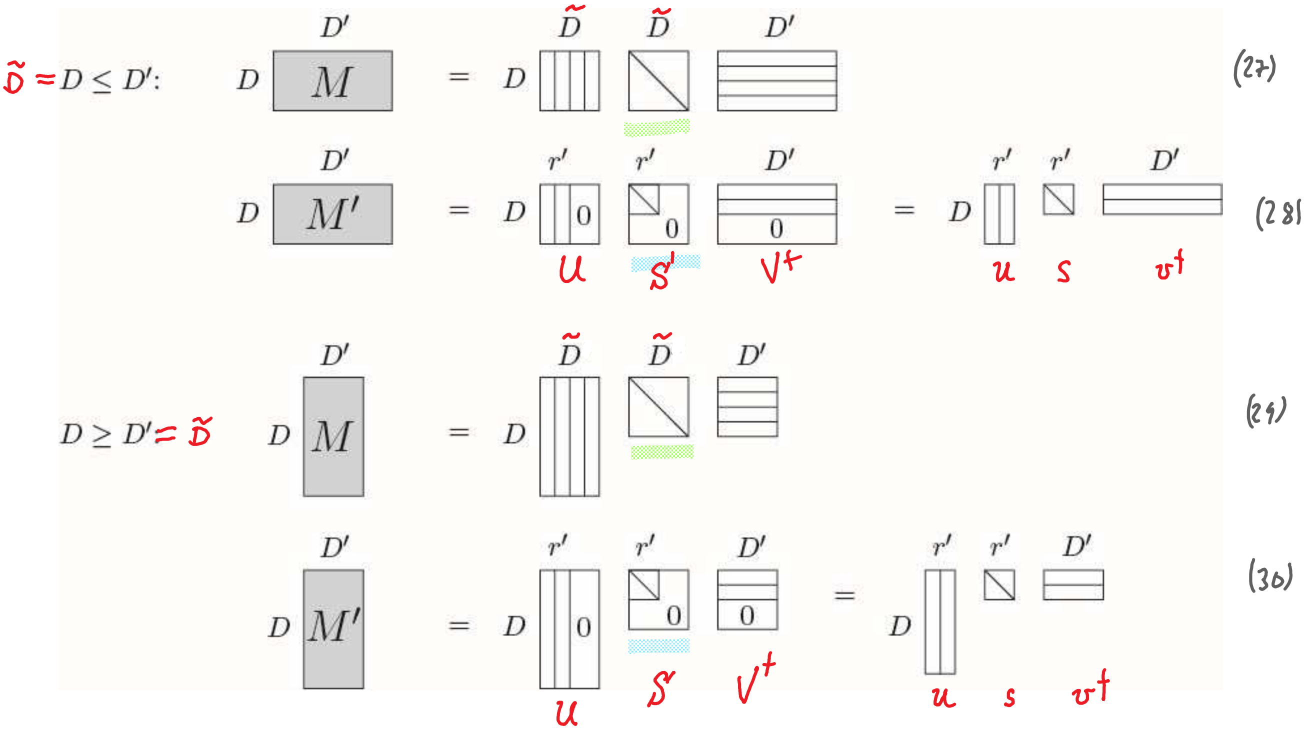
Truncate: $\boxed{M' := U S' V^\dagger}$ (25)

with $S' := \mathrm{diag}(s_1, s_2, \ldots, s_{r'}, \underbrace{0, \ldots, 0, \ldots, 0}_{\tilde D - r' \text{ zeros}})$ (26)



Retain only r' largest singular values!

Visualization, with $r = \tilde D$:



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

in the sense that it can be shown to minimize the Frobenius norm of the difference, $M - M'$.

$$\|M - M'\|_F^2 = \mathrm{Tr}\,(M - M')^\dagger (M - M') = \mathrm{Tr}\,(M^\dagger M + M'^\dagger M' - M'^\dagger M - M^\dagger M') \quad (31)$$

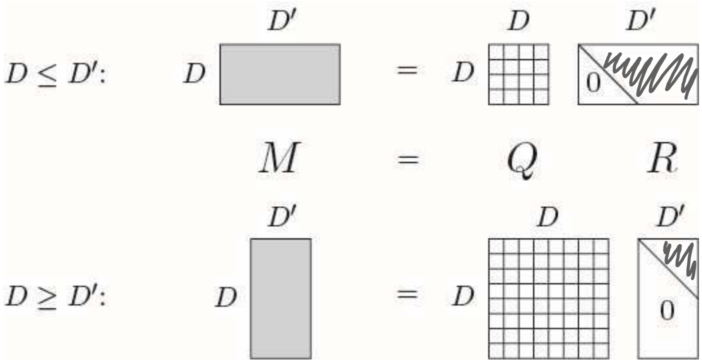
similar steps as for (8)

$$= \mathrm{Tr}\,(S\cdot S + S'\cdot S' - \underbrace{S'\cdot S}_{= S'\cdot S'} - \underbrace{S\cdot S'}_{= S'\cdot S'}) \quad (32)$$

$$= \mathrm{Tr}\left(S^2 - S'^2 \right) = \sum_{\alpha=1}^{r} s_\alpha^2 - \sum_{\alpha=1}^{r'} s_\alpha^2 = \boxed{\sum_{\alpha=r'+1}^{r} s_\alpha^2} \qquad (33)$$

'discarded weight'

QR-decomposition



If singular values are not needed,

a $D \times D'$ matrix M

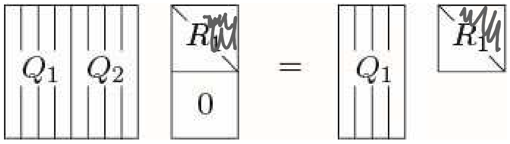
has the 'full QR decomposition'

$$M = QR \qquad (14)$$

with Q a $D \times D$ unitary matrix, $QQ^\dagger = Q^\dagger Q = \mathbb{1}$ (29)

and R a $D \times D'$ upper triangular matrix, $R_{\alpha\beta} = 0$ if $\alpha > \beta$ (30)

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



$$M = (Q_1, Q_2) \cdot \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 \cdot R_1 \qquad (17)$$

with dim(Q1) = $D \times D'$, dim(R1) = $D' \times D'$, $Q_1^\dagger Q_1 = \mathbb{1}$ but $Q_1 Q_1^\dagger \neq \mathbb{1}$ (31)

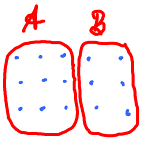
and R1 upper triangular.

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

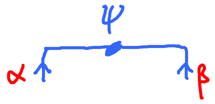
3. Schmidt decomposition

[most efficient way of representing entanglement]

Consider a quantum system composed of two subsystems, $\mathcal{A}$ and $\mathcal{B}$, with orthonormal bases $\{|\alpha\rangle_{\mathcal{A}}\}$ and $\{|\beta\rangle_{\mathcal{B}}\}$.



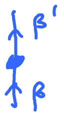
Pure state on $\mathcal{A} \cup \mathcal{B}$: $|\psi\rangle = |\beta\rangle_{\mathcal{B}} |\alpha\rangle_{\mathcal{A}} \psi^{\alpha\beta}$ (1)



Reduced density matrices of subsystems $\mathcal{A}$ and $\mathcal{B}$:

$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}} |\psi\rangle\langle\psi| = |\alpha\rangle_{\mathcal{A}} (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} \, {}_{\mathcal{A}}\langle\alpha'|$, $\quad (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'}$ (2)

$\hat{\rho}_{\mathcal{B}} = \mathrm{Tr}_{\mathcal{A}} |\psi\rangle\langle\psi| = |\beta\rangle_{\mathcal{B}} (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} \, {}_{\mathcal{B}}\langle\beta'|$, $\quad (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} = (\psi^{\dagger}\psi)_{\beta'}{}^{\beta}$ (3)

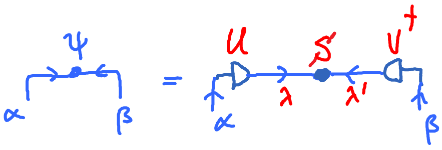


Singular value decomposition

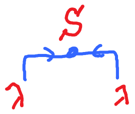
Use SVD to find bases for $\mathcal{A}$ and $\mathcal{B}$ which diagonalize density matrices:

$$\psi \overset{\text{SVD}}{=} U S V^{\dagger} \quad (4)$$

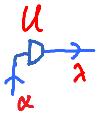
With indices: $\psi^{\alpha\beta} = U^{\alpha}{}_{\lambda} \underset{\uparrow \, \mathrm{diag}(s_1, s_2, \dots)}{S^{\lambda\lambda'}} V^{\dagger}{}_{\lambda'}{}^{\beta}$ (5)



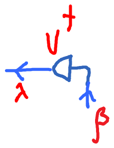
Hence $|\psi\rangle = |\lambda'\rangle_{\mathcal{B}} |\lambda\rangle_{\mathcal{A}} S^{\lambda\lambda'} = \sum_{\lambda} |\lambda\rangle_{\mathcal{B}} |\lambda\rangle_{\mathcal{A}} s_{\lambda}$ (6)



where $|\lambda\rangle_{\mathcal{A}} = |\alpha\rangle_{\mathcal{A}} U^{\alpha}{}_{\lambda}$,



; $|\lambda\rangle_{\mathcal{B}} = |\beta\rangle V^{\dagger}{}_{\lambda}{}^{\beta}$,

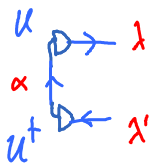


(7)

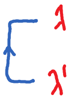
are orthonormal sets of states for $\mathcal{A}$ and $\mathcal{B}$, and can be extended to yield orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$ if needed.

Orthonormality is guaranteed by $U^{\dagger} U = \mathbb{1}$ and $V^{\dagger} V = \mathbb{1}$! (8)

${}_{\mathcal{A}}\langle\lambda'|\lambda\rangle_{\mathcal{A}} =$

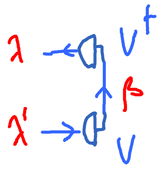


$= U^{\dagger\lambda'}{}_{\alpha} U^{\alpha}{}_{\lambda} = \mathbb{1}^{\lambda'}{}_{\lambda} =$

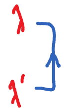


(9)

${}_{\mathcal{B}}\langle\lambda'|\lambda\rangle_{\mathcal{B}} =$



$= V^{\dagger}{}_{\lambda}{}^{\beta} V_{\beta}{}^{\lambda'} = \mathbb{1}_{\lambda}{}^{\lambda'} =$



(10)

Restrict $\sum_{\lambda}$ to the r non-zero singular values:

$|\psi\rangle = \sum_{\lambda=1}^{r} |\lambda\rangle_{\mathcal{B}} |\lambda\rangle_{\mathcal{A}} s_{\lambda}$ 'Schmidt decomposition' (11)

If $r = 1$, 'classical' state: $|\psi\rangle = |1\rangle_B |1\rangle_A$.   If $r \geq 1$: 'entangled state'

In this representation, reduced density matrices are diagonal:

$$\hat{\rho}_A = \mathrm{Tr}_B |\psi\rangle\langle\psi| = \sum_\lambda |\lambda\rangle_A (s_\lambda)^2 \, {}_A\langle\lambda| \tag{12}$$

$$(\psi\psi^\dagger), (\psi^\dagger\psi) \quad \text{with} \quad \psi^{\lambda\lambda'} = S_\lambda \mathbb{1}^{\lambda\lambda'} \tag{13}$$

$$\hat{\rho}_B = \mathrm{Tr}_A |\psi\rangle\langle\psi| = \sum_\lambda |\lambda\rangle_B (s_\lambda)^2 \, {}_B\langle\lambda| \tag{14}$$

Entanglement entropy:
$$S_{A|B} = - \sum_{\lambda=1}^{r} (s_\lambda)^2 \ln_2 (s_\lambda)^2 \tag{15}$$

Note: for given r , entanglement is maximal if all singular values are equal, $S_\lambda = r^{-1/2}$ (16)

How can one approximate $|\psi\rangle = \sum_{\alpha\beta} |\beta\rangle_B |\alpha\rangle_A \psi^{\alpha\beta}$ by cheaper $|\tilde{\psi}\rangle$?

$$\| |\psi\rangle \|_2^2 \equiv |\langle\psi|\psi\rangle|^2 = \sum_{\alpha\beta} |\psi^{\alpha\beta}|^2 = \|\psi\|_F^2 \tag{17}$$

Define truncated state using r' $(< r)$ singular values:

$$|\tilde{\psi}\rangle \equiv \sum_{\lambda=1}^{r'} |\lambda\rangle_B |\lambda\rangle_A \, s_\lambda \tag{18}$$

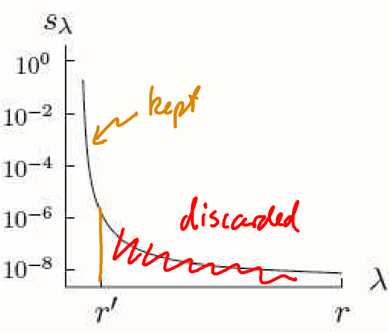
If $|\tilde{\psi}\rangle$ should be normalized, rescale, i.e. replace S_λ by $S_\lambda \left[\sum_{\lambda'=1}^{r'} (s_{\lambda'})^2 \right]^{-1/2}$ (19)

Truncation error:

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|_2^2 = \langle\psi|\psi\rangle + \langle\tilde{\psi}|\tilde{\psi}\rangle - 2 \, \mathrm{Re} \langle\tilde{\psi}|\psi\rangle$$

$$= \sum_{\lambda=1}^{r} (s_\lambda)^2 + \sum_{\lambda=1}^{r'} (s_\lambda)^2 - 2 \sum_{\lambda=1}^{r'} (s_\lambda)^2 = \sum_{\lambda=r'+1}^{r} (s_\lambda)^2$$

= sum of squares of discarded singular values



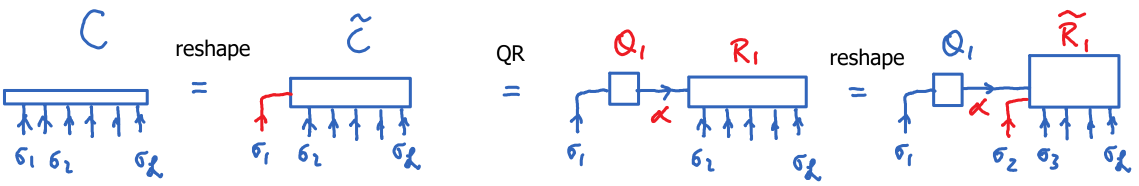
Useful to obtain 'cheap' representation of $|\psi\rangle$ if singular values decay rapidly.

The truncation strategy (18) minimizes the truncation error.
It is used over and over again in tensor network numerics.

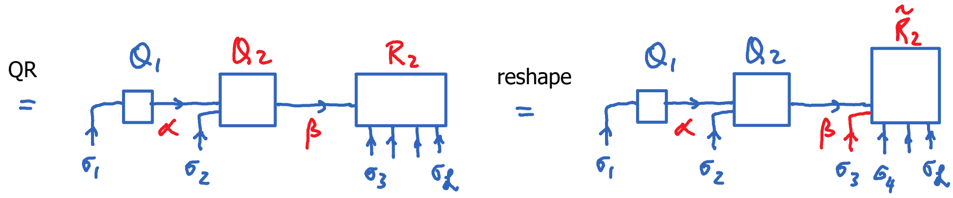
4. Reshaping generic tensor into MPS form

TNB-III.4

A generic tensor of arbitrary rank can be expressed as an MPS by repeatedly performing SVDs.



(1)



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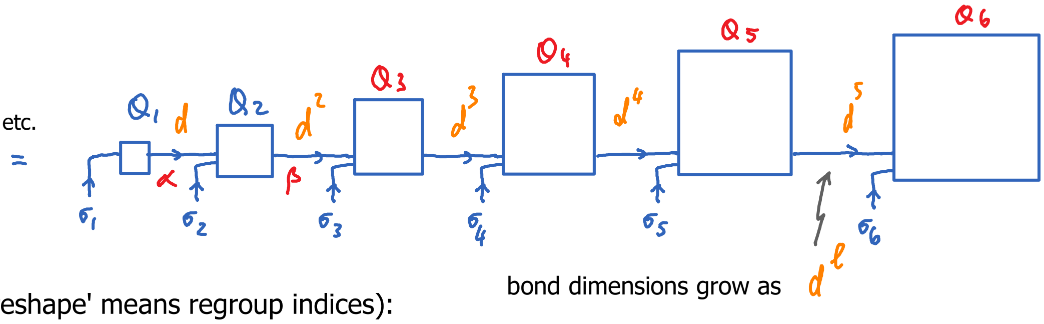


(3)

In formulas ('reshape' means regroup indices):

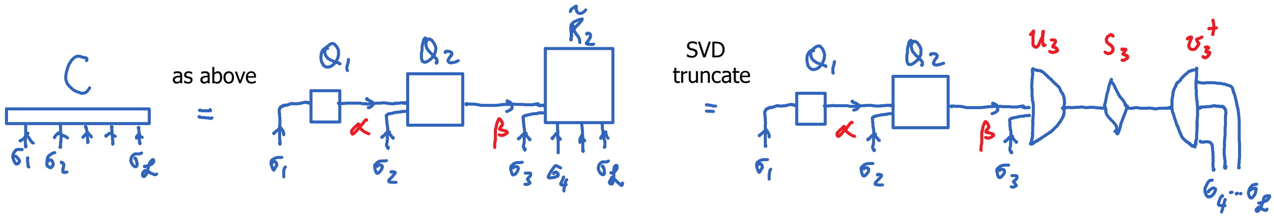
$$C^{\sigma_1\cdots\sigma_N} \overset{\text{reshape}}{=} \tilde{C}^{\sigma_1,\sigma_2\ldots\sigma_\ell} \overset{\text{QR}}{=} Q_1^{\sigma_1}{}_{\alpha} R_1^{\alpha,\sigma_2\ldots\sigma_\ell} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_{\alpha} \tilde{R}_1^{\alpha\sigma_2,\sigma_3\ldots\sigma_\ell} \quad (4)$$

$$\overset{\text{QR}}{=} Q_1^{\sigma_1}{}_{\alpha} Q_2^{\alpha\sigma_2}{}_{\beta} R_2^{\beta,\sigma_3\ldots\ell} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_{\alpha} Q_2^{\alpha\sigma_2}{}_{\beta} \tilde{R}_2^{\beta\sigma_3,\sigma_4\cdots\ell} = \ldots \quad \text{etc.} \quad (5)$$

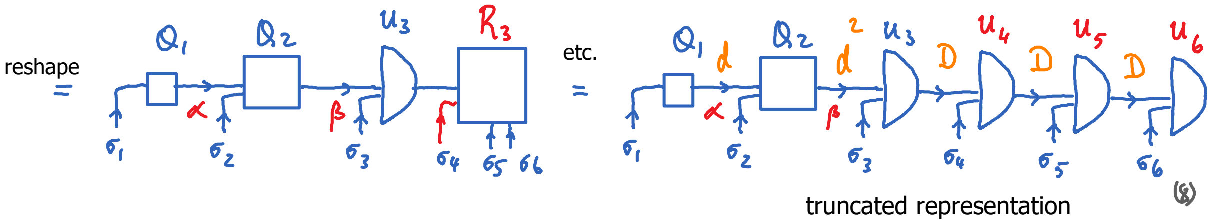
$$= Q_1^{\sigma_1}{}_{\alpha} Q_2^{\alpha\sigma_2}{}_{\beta} Q_3^{\beta\sigma_3}{}_{\gamma} \cdots R_{\ell-1}^{\mu\sigma_\ell} \quad (6)$$

If a maximal bond dimension of $D_\alpha < D$ is desired, this can be achieved using SVD instead of QR decompositions, and truncating by retaining only largest D singular values at each step:

$R \overset{\text{SVD}}{=} USV^\dagger \overset{\text{truncate}}{\simeq} usv^\dagger$ where s contains only largest D singular values of S



(7)



(8)