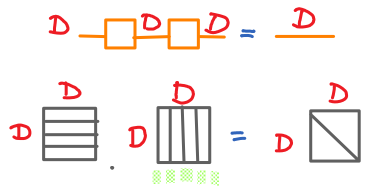
4. Unitaries and isometries

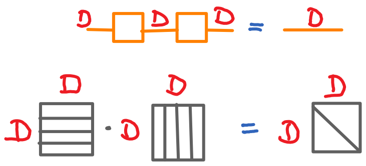
TNB.4

Unitaries (unitary = invertible distance-preserving linear map)

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

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

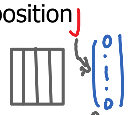




Its column vectors, $U = (\vec{u}_1, \vec{u}_2, \dots, \vec{u}_D)$, form a basis for $\mathbb{C}^D$ (2)

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 $\mathbb{C}^D$

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

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

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

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

consistent with (3b)

Left isometry (isometry = distance-preserving linear map, not necessarily invertible)

A rectangular matrix $A \in \mathrm{mat}(D, D'; \mathbb{C})$ with $D \geq D'$ is called a 'left isometry' if (6a) holds:

$$\boxed{A^\dagger A = \mathbb{1}_{D'} \quad (6a) \qquad \text{Note: if } D > D' \text{ then } \quad A A^\dagger \neq \mathbb{1}} \qquad (6b)$$

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)

$$\vec{a}_i^{\,\dagger} = \bar{\vec{a}}_i^{\,T}$$

They form a basis for a D'-dimensional (sub)space of $\mathbb{C}^D$ ← space of D-dimensional column vectors

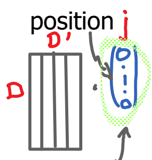
$u \quad - \quad u_1$

They form a basis for a D'-dimensional (sub)space of $\mathbb{C}^D$, space of D-dimensional column vectors

say $V_A = \mathrm{span}\{\vec a_1, \vec a_2, \dots, \vec a_{D'}\}$ $\begin{cases} \subsetneq \mathbb{C}^D & \text{true subspace if } D' < D \\ = \mathbb{C}^D & \text{if } D' = D \end{cases}$ (8)

[The D row vectors of A each are elements of $\mathbb{C}^{\times D'}$, not $\mathbb{C}^{\times D}$]

dual space of D'-dimensional row vectors

A defines an isometric map:  $= \Big| = \vec a_j \in \mathbb{C}^D$, $j = 1, \dots, D'$ (9a)

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

Formally:

$\boxed{A : \mathbb{C}^{D'} \to \mathbb{C}^D}$,

short column vectors — long column vectors

$\vec f_j \mapsto A \vec f_j := \vec e_i A^i{}_j = \vec a_j$ (short, long, long) $j \in 1, \dots, D'$ (9b)

standard basis vector in $\mathbb{C}^D$ $\quad i \in 1, \dots, D$

(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 A', with dimension $\dim(A) = D'$.

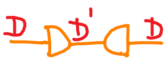
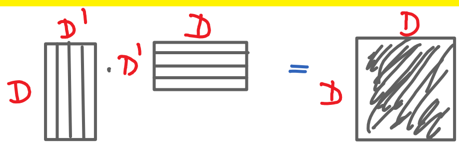
because A has fewer columns than rows

<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

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

<u>Left projector</u>

 $= P = A A^\dagger =$  (11)

is a projector, since $P^2 = (A \underbrace{A^\dagger)(A}_{(6a)\ \mathbb{1}_{D'}} A^\dagger) = A A^\dagger = P$ (12)

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

$$P \vec a_j \overset{(11, 9b)}{=} A \underbrace{A^\dagger A}_{(6a) = \mathbb{1}_{D'}} \vec f_j = A \vec f_j \overset{(9b)}{=} \vec a_j$$

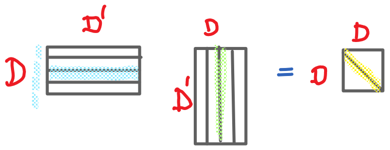
Right isometry

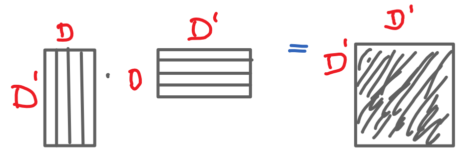
A rectangular matrix $B \in \mathrm{mat}(D, D'; \mathbb{C})$ with $D \le D'$ is called a 'right isometry' if (14a) holds:

D — D'

$$B B^\dagger = \mathbb{1}_D \quad (14a) \qquad \text{Note: if } D < D' \text{ then} \quad B^\dagger B \neq \mathbb{1}_{D'} \quad (14b)$$

D — D' — D $=$ D $\qquad$ D' — D — D'





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)

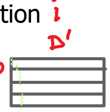
[row vectors (dual to column vectors) are labeled using upstairs index]

space of D'-dimensional row vectors

They form a basis for a D-dimensional (sub)space of $\mathbb{C}^{D'*}$,

say $V_B^* = \mathrm{span}\{\vec b^1, \vec b^2, \dots, \vec b^D\}$ $\begin{cases} \subsetneq \mathbb{C}^{D'*} & \text{true subspace if } D < D' \\ = \mathbb{C}^{D'*} & \text{if } D = D' \end{cases}$ (16)

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

B defines an isometric map: $(0 \dots 1 \dots 0) \cdot$  $=$ row i $=$ $\vec b^i \in \mathbb{C}^{D'*}$, $i = 1, \dots, D$ (17a)

position i, D', D

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

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

short row vectors $\qquad$ 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.

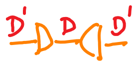
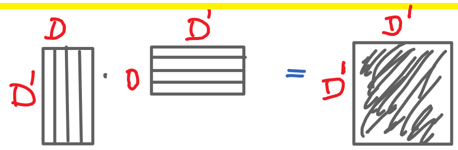
These span $V_B^* \subseteq \mathbb{C}^{D'*}$, the 'image space of B' or 'image of B', with dimension $\dim(B) = D$.
$\subsetneq$ if B has fewer rows than columns

Invariance of scalar product (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

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

Right projector

 $= P = B^\dagger B =$  (19)

is a projector, since $P^2 = (B^\dagger \underbrace{B)(B^\dagger}_{\overset{(14a)}{\mathbb{1}_D}} B) = B^\dagger B = P$ (20)

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

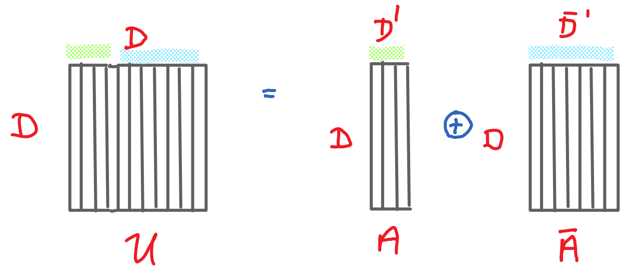
$$\vec{b}^{\,i} P \overset{(19,17b)}{=} \vec{f}^{\,i} \underbrace{B\, B^\dagger}_{(14a)=\mathbb{1}} B = \vec{f}^{\,i} B \overset{(17b)}{=} \vec{b}^{\,i} \quad ✓ \tag{21}$$

Truncation of unitaries yield isometries

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

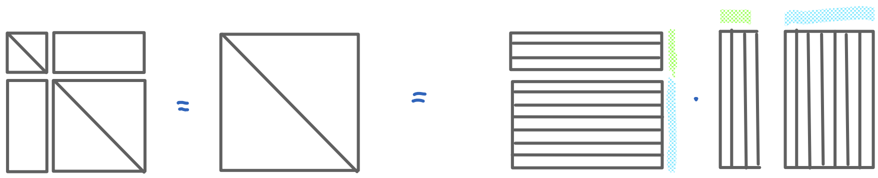
and partition its columns into two groups, containing D' and $\bar{D}' = D - D'$ columns:

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

 (24)

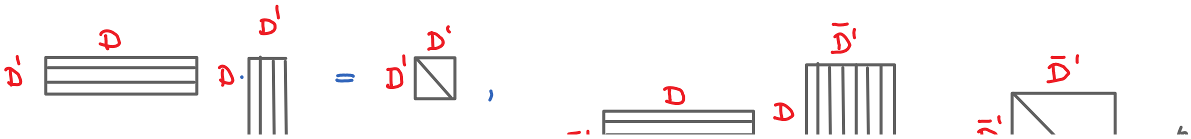
Unitarity of U implies:

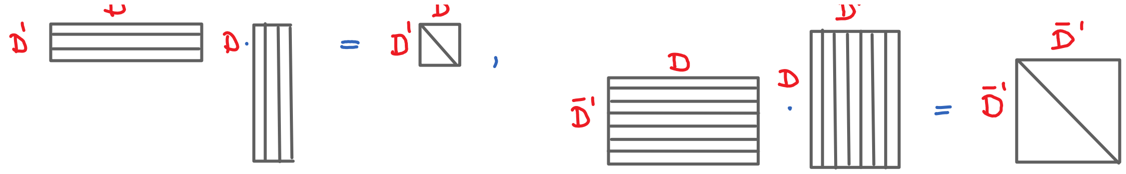
$$\begin{pmatrix} \mathbb{1}_{D'} & 0 \\ 0 & \mathbb{1}_{\bar{D}'} \end{pmatrix} = \mathbb{1}_D = U^\dagger U = \begin{pmatrix} A^\dagger \\ \bar{A}^\dagger \end{pmatrix} (A \,,\, \bar{A}) = \begin{pmatrix} A^\dagger A & A^\dagger \bar{A} \\ \bar{A}^\dagger A & \bar{A}^\dagger \bar{A} \end{pmatrix} \tag{25}$$

 (26)

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

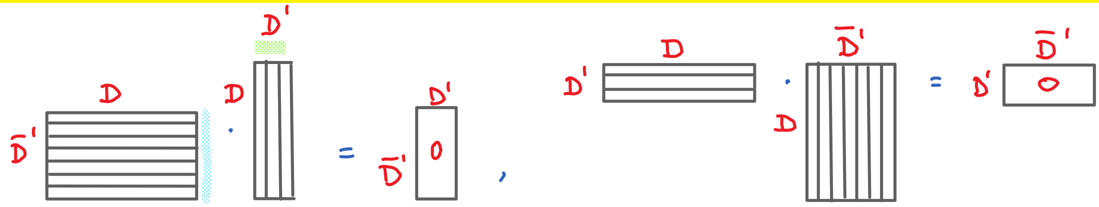
 $= A^\dagger A \overset{(25)}{=} \mathbb{1}_{D'}$,  $= \bar{A}^\dagger \bar{A} \overset{(25)}{=} \mathbb{1}_{\bar{D}'}$ (27)



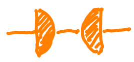

(28)

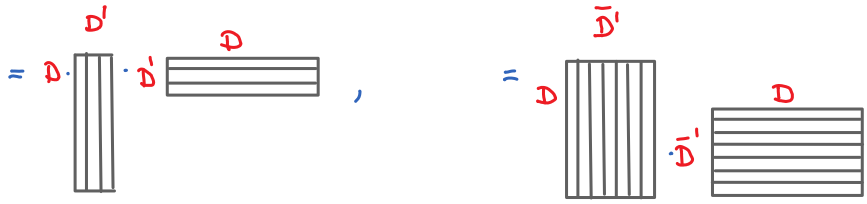
Moreover, A are $\bar{A}$ orthogonal to each other, since they are built from orthogonal column vectors:

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

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

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:

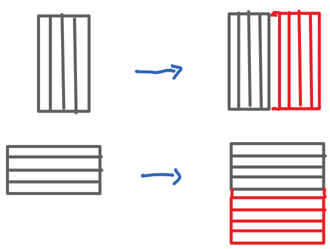
$$P : \mathbb{C}^D \to V_A = \mathrm{span}\{\vec{u}_1, \dots \vec{u}_{D'}\} =: \mathrm{span}\{\vec{a}_1, \dots, \vec{a}_{D'}\} \subsetneq \mathbb{C}^D \tag{35}$$

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

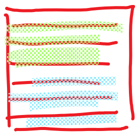
with $\vec{x}^\dagger \cdot \vec{y} = 0 \quad \forall \ \vec{x} \in V_A \ , \ \vec{y} = V_{\bar{A}}$ (37)

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)

A discussion similar to the above holds for splitting a unitary matrix into two sets of rows, yielding two right isometries.

$U =$  $= \begin{pmatrix} B \\ \bar{B} \end{pmatrix}$

$$B B^\dagger = \mathbb{1} \qquad B \bar{B}^\dagger = 0$$

$$\bar{B} \bar{B}^\dagger = \mathbb{1} \qquad \bar{B} B^\dagger = 0$$

5. Singular value decomposition (SVD)

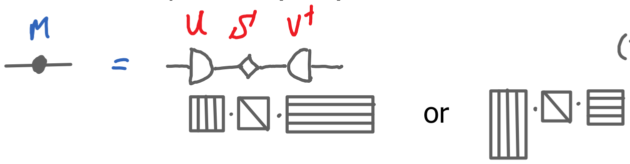
[Schollwoeck2011, Sec. 4] TNB.5

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)

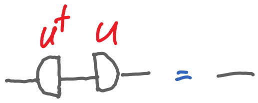
Theorem: Any such M has a singular value decomposition (SVD) of the form

$$\boxed{M = U \cdot S \cdot V^\dagger} \tag{2}$$

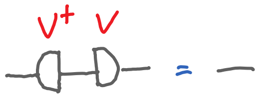


where

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



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



$S \in \mathrm{mat}(\tilde{D}, \tilde{D}; \mathbb{R})$ is diagonal, with real, non-negative diagonal elements, called 'singular values' (5)

Remarks:

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

$$MM^\dagger \overset{(2)}{=} (USV^\dagger)(VSU^\dagger) \overset{(4)}{=} US^2U^\dagger \overset{(3)}{\Rightarrow} \quad MM^\dagger U = US^2 \tag{6}$$

$$M^\dagger M \overset{(2)}{=} (VSU^\dagger)(USV^\dagger) \overset{(3)}{=} VS^2V^\dagger \overset{(4)}{\Rightarrow} \quad M^\dagger M V = VS^2 \tag{7}$$

So, eigenvectors of $MM^\dagger$ yield columns of U, eigenvectors of $M^\dagger M$ yield columns of .
They have the same set of eigenvalues, yielding the squares of the singular values.

(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' $:= S_{\alpha\alpha} =$ $\tilde{D}$

- '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)

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

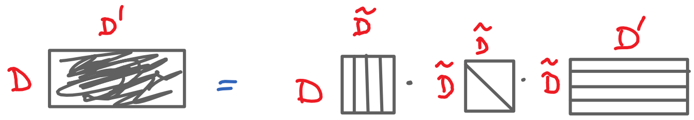
(iii) Properties of U and $V^\dagger$: $\tilde{D} = \min(D, D')$

- $\dim(U) = D \times \tilde{D}$, $\boxed{U^\dagger U = \mathbb{1}_{\tilde{D}}}$, 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 $\tilde{D} = D \leq D'$:

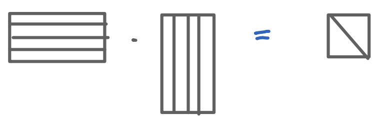


$$M = \ldots = U \cdot S \cdot V^\dagger \qquad (15)$$

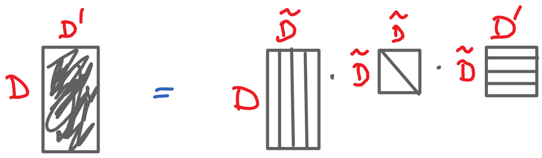
U is unitary: $U^\dagger U = \ldots = \mathbb{1}$ (16)

product is arranged such that the outer indices have the smallest dimension,

$V^\dagger$ is right isometry: $V^\dagger V = \ldots = \mathbb{1}$ (17)

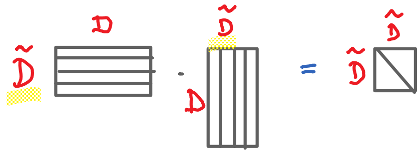


If $D \geq D' = \tilde{D}$:



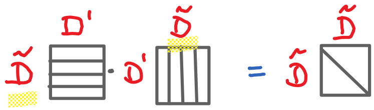
$$M = \ldots = U \cdot S \cdot V^\dagger \qquad (18)$$

U is left isometry: $U^\dagger U = \ldots = \mathbb{1}_{\tilde{D}}$ (19)



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

$V^\dagger$ is unitary: $V^\dagger V = \ldots = \mathbb{1}_{\tilde{D}}$ (20)



(vi) Truncation via SVD

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

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

trace is cyclic

singular values determine norm

<u>Truncation</u>

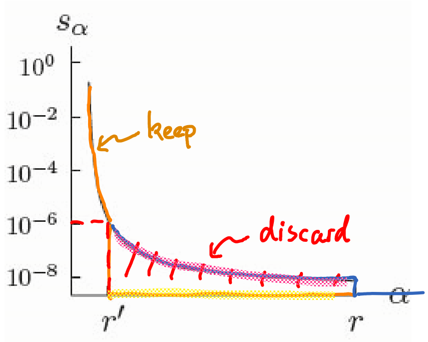
SVD can be used to approximate a rank r matrix M by a rank r' $(<r)$ matrix M' :

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

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

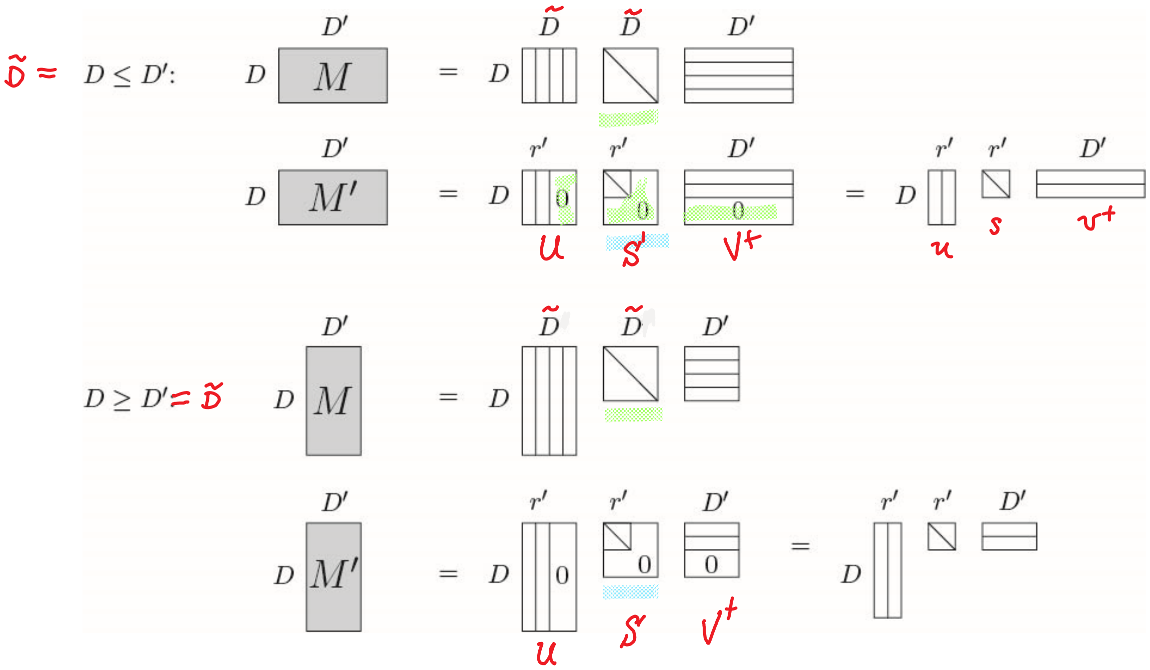
Truncate: $\boxed{M' := U S' V^\dagger}$ (25)

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



Retain only r' largest singular values!

Visualization, with $r = \tilde{D}$:



(27)

(28)

(29)

(30)

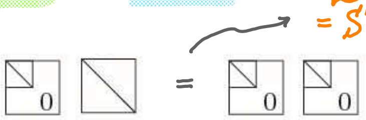
SVD truncation yields 'optimal' approximation of a rank r matrix M by a rank r' $(<r)$ matrix M',

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

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

similar steps as for (8)

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



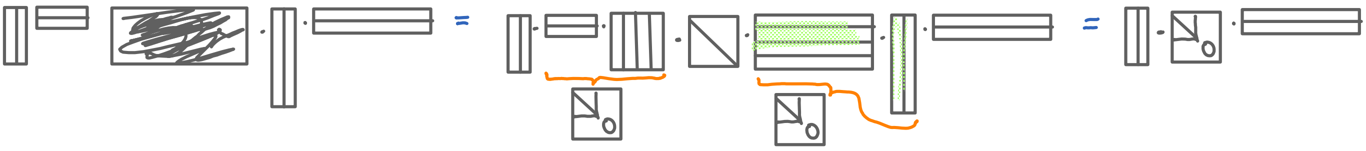
'discarded weight'

'discarded weight'

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

Note:

$$u u^\dagger M v v^\dagger = u u^\dagger \, U S V^\dagger \, v v^\dagger = u s v^\dagger = M'$$



(vi) Polar decomposition of square matrix

no negative eigenvalues

Any square matrix can be factored into a Hermitian, positive matrix and a unitary matrix:

$$M = U S V^\dagger = \begin{cases} (U S U^\dagger)(U V^\dagger) = P W & \text{'left polar decomposition'} \\ (U V^\dagger)(V S V^\dagger) = \tilde{W} \tilde{P} & \text{'right polar decomposition'} \end{cases} \qquad (34)$$

This generalizes the polar decomposition for complex numbers, $z = |z| e^{i\phi}$

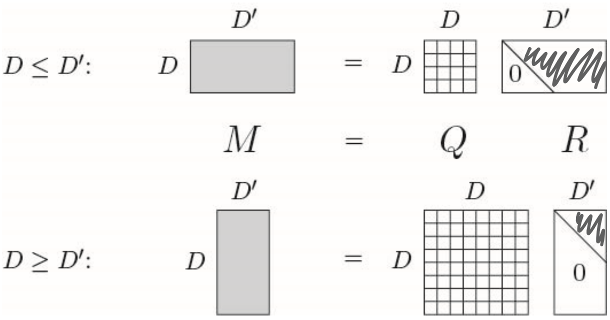
QR-decomposition

If singular values are not needed,

a $D \times D'$ matrix M

has the 'full QR decomposition'

$$M = QR \qquad (35)$$

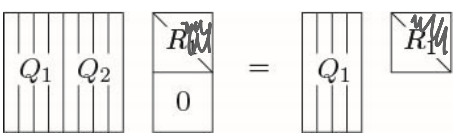


with Q a $D \times D$ unitary matrix, $\qquad QQ^\dagger = Q^\dagger Q = \mathbb{1} \qquad (36)$

and R a $D \times D'$ upper triangular matrix, $\qquad R_{\alpha\beta} = 0$ if $\alpha > \beta \qquad (37)$

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

$$M = (Q_1, Q_2) \cdot \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 \cdot R_1 \qquad (38)$$



with dim(Q1) = $D \times D'$, dim(R1) = $D' \times D'$, and R1 upper triangular.

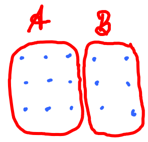
$$Q_1^\dagger Q_1 = \mathbb{1} \quad \text{but} \quad Q_1 Q_1^\dagger \neq \mathbb{1} \qquad (39)$$

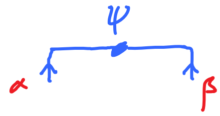
QR-decomposition is numerically cheaper than SVD, but has less information (not 'rank-revealing').

6. Schmidt decomposition [most efficient way of representing entanglement]

TNB.6

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

Reduced density matrices of subsystems $\mathcal{A}$ and $\mathcal{B}$: $\quad \mathrm{Tr}_{\mathcal{B}}\,|\beta\rangle\langle\beta'| = \delta_{\beta}{}^{\beta'}$

$$\hat{\rho}_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}\,|\psi\rangle\langle\psi| = \mathrm{Tr}_{\mathcal{B}}\,\psi^{\alpha\beta}|\alpha\rangle_{\mathcal{A}}|\beta\rangle_{\mathcal{B}}\;{}_{\mathcal{B}}\langle\beta'|\,{}_{\mathcal{A}}\langle\alpha'|\,\overline{\psi_{\alpha'\beta'}} = |\alpha\rangle_{\mathcal{A}}\,\psi^{\alpha\beta}\,\overline{\psi_{\beta\alpha'}}\;{}_{\mathcal{A}}\langle\alpha'| \qquad (2)$$

$$= |\alpha\rangle_{\mathcal{A}}\,(\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'}\;{}_{\mathcal{A}}\langle\alpha'|, \qquad \text{with} \qquad (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'} \qquad (3)$$

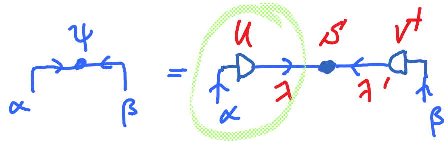
Singular value decomposition

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

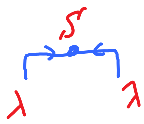
$$\psi \overset{\text{SVD}}{=} U S V^{\dagger} \qquad (4)$$

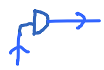
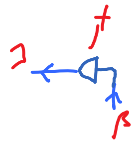
With indices: $\quad \psi^{\alpha\beta} = U^{\alpha}{}_{\lambda}\,S^{\lambda\lambda'}\,V^{\dagger}{}_{\lambda'}{}^{\beta}$

S = diag$(s_1, s_2, \ldots)$



(5)

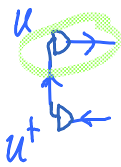
Hence $\quad |\psi\rangle = |\lambda'\rangle_{\mathcal{A}}|\lambda\rangle_{\mathcal{B}}\,S^{\lambda\lambda'} = \sum_{\lambda}|\lambda\rangle_{\mathcal{A}}|\lambda\rangle_{\mathcal{B}}\,s_{\lambda}$  (6)

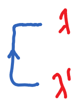
where $\quad |\lambda\rangle_{\mathcal{A}} = |\alpha\rangle_{\mathcal{A}}\,U^{\alpha}{}_{\lambda}$,  ; $\quad |\lambda\rangle_{\mathcal{B}} = |\beta\rangle\,V^{\dagger}{}_{\lambda}{}^{\beta}$,  (7)

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.

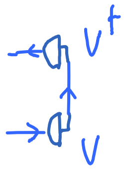
Orthonormality is guaranteed by $\quad U^{\dagger}U = \mathbb{1}$ and $V^{\dagger}V = \mathbb{1}$! (8)

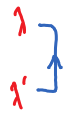
$${}_{\mathcal{A}}\langle\lambda'|\lambda\rangle_{\mathcal{A}} = \text{[diagram]} = U^{\dagger\lambda'}{}_{\alpha}\,U^{\alpha}{}_{\lambda} = \mathbb{1}^{\lambda'}{}_{\lambda} = \text{[diagram]} \qquad (9)$$





$${}_{\mathcal{B}}\langle\lambda'|\lambda\rangle_{\mathcal{B}} = \text{[diagram]} = V^{\dagger}{}_{\lambda}{}^{\beta}\,V_{\beta}{}^{\lambda'} = \mathbb{1}_{\lambda}{}^{\lambda'} = \text{[diagram]} \qquad (10)$$





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

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

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

In this representation, reduced density matrices are diagonal:

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

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

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

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

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

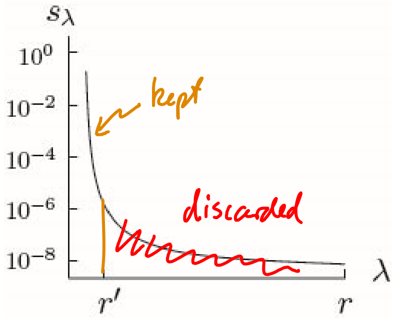
Then,
$$S_{A|B} = \ln r \qquad \text{(this proves (TNB1.13)} \qquad (16)$$

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

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

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

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



Truncation error:

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

$$= \sum_{\lambda=1}^{r} (s_\lambda)^2 + \sum_{\lambda=1}^{r'} (s_\lambda)^2 - 2\sum_{\lambda=1}^{r'} (s_\lambda)^2 = \sum_{\lambda=r'+1}^{r} (s_\lambda)^2 \qquad (19)$$

$=$ sum of squares of discarded singular values = 'discarded weight'

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

If $|\tilde{\psi}\rangle$ should be normalized, rescale, i.e. replace s_λ by
$$s_\lambda \left[\sum_{\lambda'=1}^{r'} (s_{\lambda'})^2 \right]^{-1/2} \qquad (20)$$

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