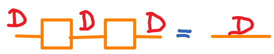
4. Unitaries and isometries

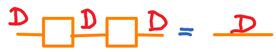
TNB.4

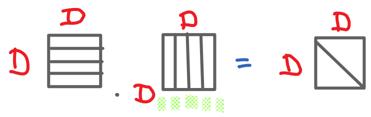
Unitaries (unitary = invertible distance-preserving linear map)

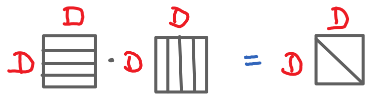
A square matrix $U \in \mathrm{mat}(D, D; \mathbb{C})$ is called 'unitary' if it satisfies:

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









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 $\mathbb{C}^D$

U defines an invertible map: position j column j

$$\begin{array}{c}\text{position } j \quad \text{column } j\end{array}$$

$$U \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \Big| = \vec{u}_j \in \mathbb{C}^D, \quad j = 1, \dots, D \quad (3a)$$

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

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

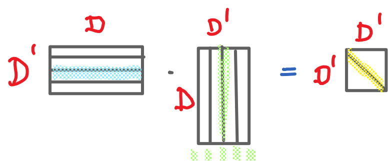
Indeed, then $U^\dagger \vec{u}_j \overset{(3b)}{=} U^\dagger \vec{e}_i \, U^i{}_j \overset{(4)}{=} \vec{e}_k \underbrace{U^{\dagger k}{}_i \, U^i{}_j}_{(1a) = \delta^k{}_j} = \vec{e}_j$ ✓ (5)

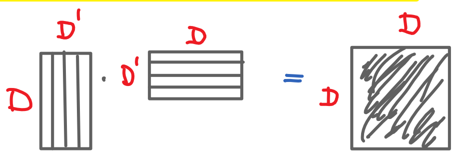
consistent with (3b)

Left isometry (isometry = distance-preserving 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:

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





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)

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

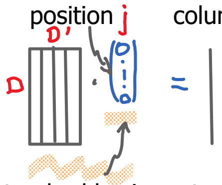
They form a basis for a D'-dimensional (sub)space of $\mathbb{C}^D$ ← space of D-dimensional column vectors

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

say $\boxed{V_A = \mathrm{span}\{\vec{a}_1, \vec{a}_2, \dots, \vec{a}_{D'}\} \begin{cases} \subsetneq \mathbb{C}^D & \text{true subspace if } D' < D \\ = \mathbb{C}^D & \text{if } D' = D \end{cases}}$ (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:



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

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

Formally:

$\boxed{A : \underset{\substack{\text{short}\\\text{column}\\\text{vectors}}}{\mathbb{C}^{D'}} \to \underset{\substack{\text{long}\\\text{column}\\\text{vectors}}}{\mathbb{C}^{D}}}$, $\quad \vec{f}_j \mapsto A\vec{f}_j := \vec{e}_i A^i{}_j = \vec{a}_j \quad$ $j \in 1, \dots, D'$, $i \in 1, \dots, D$ (9b)

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 A', with dimension $\dim(A) = D'$.
because A has fewer columns than rows

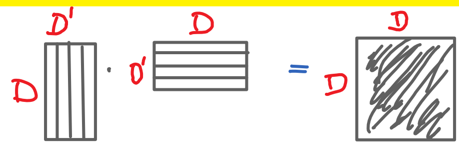
Invariance of scalar product (hence the name: iso-metric = equal metric):

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

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

Left projector

$= P = AA^\dagger =$



(11)

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

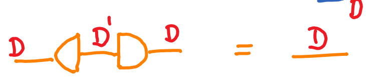
Its action leaves V_A invariant, because it leaves each of its basis vectors invariant: (13)

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

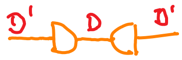
Right isometry

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

$$B B^\dagger = \mathbb{1}_D \qquad (14a)$$



Note: if $D < D'$ then $B^\dagger B \neq \mathbb{1}_{D'}$ (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]

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 $\mathbb{C}^D$, <u>not</u> $\mathbb{C}^{D'}$.]

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

$\boxed{B : \mathbb{C}^{D*} \to \mathbb{C}^{D'*}}$,
short row vectors → long row vectors

$\vec{f}^i \mapsto \vec{f}^i B := B^i{}_j\, \vec{e}^j = \vec{b}^i$ $\quad i \in 1, \dots, D;\ j \in 1, \dots, D'$ (17b)

($\vec{f}^i$: standard basis vector in $\mathbb{C}^{D*}$; $\vec{e}^j$: 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

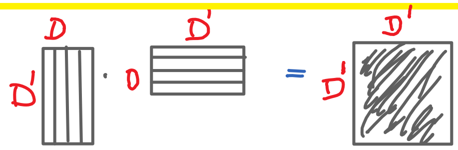
Invariance of scalar product

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

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

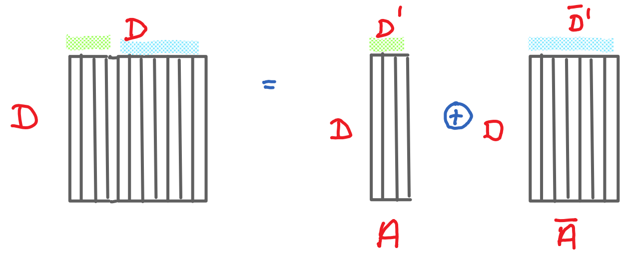
$$\vec{b}^i P \overset{(19,17b)}{=} \vec{f}^i \underbrace{B B^\dagger}_{(14a) = \mathbb{1}} B = \vec{f}^i B \overset{(17b)}{=} \vec{b}^i \quad ✓ \qquad (21)$$

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:

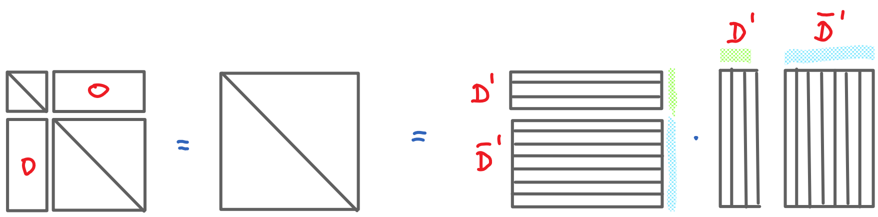
$$U = (\vec{u}_1, \vec{u}_2, \dots \vec{u}_{D'}, \vec{u}_{D'+1}, \dots \vec{u}_D) = (\vec{u}_1, \dots, \vec{u}_{D'}) \oplus (\vec{u}_{D'+1}, \dots, \vec{u}_D) =: A \oplus \bar{A} \qquad (23)$$



(24)

Unitarity of U implies:

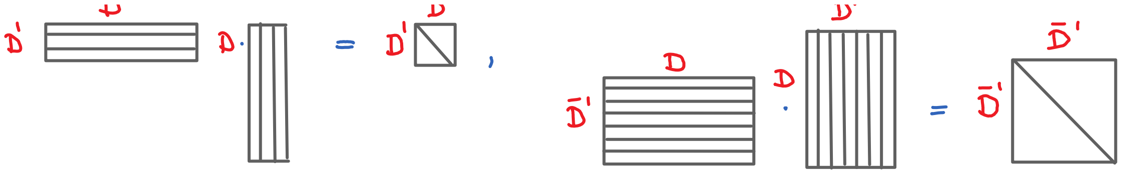
$$\begin{pmatrix} \mathbb{1}_{D'} & \\ & \mathbb{1}_{\bar{D}'} \end{pmatrix} = \mathbb{1}_D = U^\dagger U = \begin{pmatrix} A^\dagger \\ \bar{A}^\dagger \end{pmatrix} (A , \bar{A}) = \begin{pmatrix} A^\dagger A & A^\dagger \bar{A} \\ \bar{A}^\dagger A & \bar{A}^\dagger \bar{A} \end{pmatrix} \qquad (25)$$



(26)

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

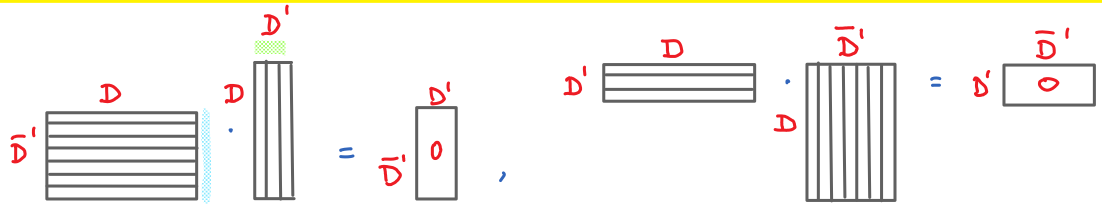
 $= A^\dagger A \overset{(25)}{=} \mathbb{1}_{D'}$,  $= \bar{A}^\dagger \bar{A} \overset{(25)}{=} \mathbb{1}_{\bar{D}'}$ (27)



(28)

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

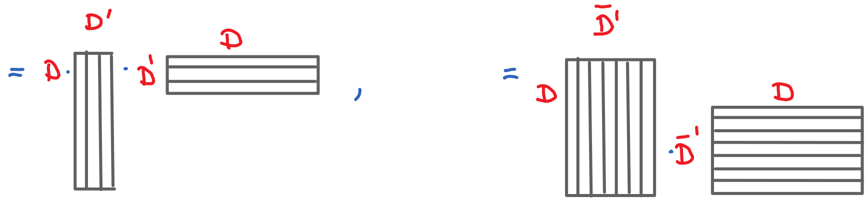
 $= \bar{A}^\dagger A \overset{(25)}{=} 0$,  $= A^\dagger \bar{A} \overset{(25)}{=} 0$ (29)



(30)

Complementary projectors

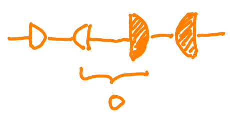
The projectors, $P = A A^\dagger =$  , $\bar{P} = \bar{A}\bar{A}^\dagger =$  (31)



are both $D \times D$ matrices,

and satisfy orthonormality relations: (32)

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

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:

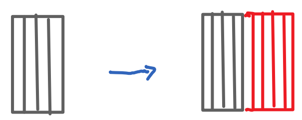
$$P : \mathbb{C}^D \to V_A = \text{span}\{\vec{u}_1, \dots \vec{u}_{D'}\} =: \text{span}\{\vec{a}_1, \dots, \vec{a}_{D'}\} \subsetneq \mathbb{C}^D \tag{35}$$

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

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.

5. Singular value decomposition (SVD)

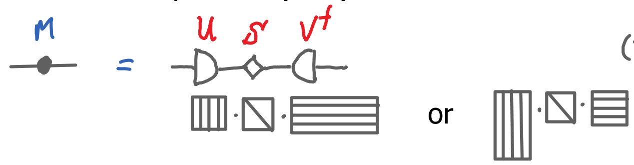
[Schollwoeck2011, Sec. 4] TNB.5

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)

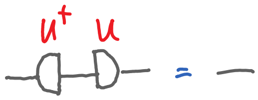
Theorem: Any such M has a singular value decomposition (SVD) of the form

$$\boxed{\underset{D\times D'}{M} = \underset{D\times\tilde{D}}{U} \cdot \underset{\tilde{D}\times\tilde{D}}{S} \cdot \underset{\tilde{D}\times D'}{V^\dagger}} \qquad (2)$$

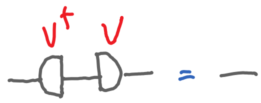


where

$U \in \mathrm{mat}(D, \tilde{D}; \mathbb{C})$ 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)



$S \in \mathrm{mat}(\tilde{D}, \tilde{D}; \mathbb{R})$ 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 $M^\dagger M$.

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

$$D'\times D':\quad M^\dagger M \overset{(2)}{=} (VS\overbrace{U^\dagger)(U}^{\mathbb{1}}SV^\dagger) \overset{(3)}{=} VS^2V^\dagger \overset{(4)}{\Rightarrow} \quad D'\times\tilde{D}:\quad M^\dagger M V = VS^2 \qquad (7)$$

So, eigenvectors of $MM^\dagger$ yield columns of U, eigenvectors of $M^\dagger M$ yield columns of V.
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' $S_\alpha := S_{\alpha\alpha} =$ $\tilde{D}$ 
- 'Schmidt rank' r : number of non-zero singular values
- arrange in descending order: $s_1 \geq s_2 \geq \dots \geq s_r > 0$ (9)

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

(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)

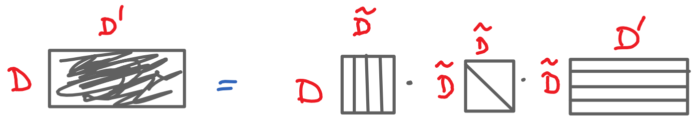
- If $D = \tilde{D}$, then U is unitary. If $D > \tilde{D}$, then U is a left isometry. (12)

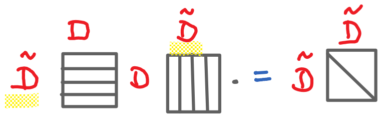
- $\dim(V^\dagger) = \tilde{D} \times D'$, $\boxed{V^\dagger V = \mathbb{1}_{\tilde{D}}}$, rows $V^\dagger$ of are orthonormal. (13)

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

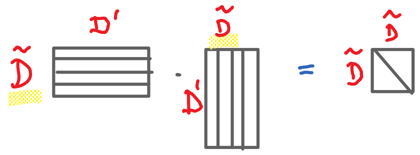
(iv) Visualization

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

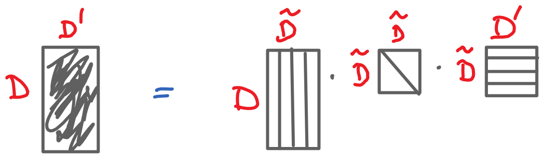
$M =$  $= U \cdot S \cdot V^\dagger$ (15)

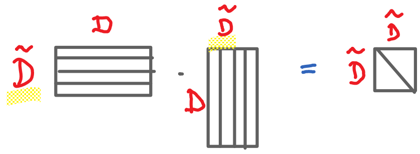
U is unitary: $U^\dagger U =$  $= \mathbb{1}_{\tilde{D}}$ (16)

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

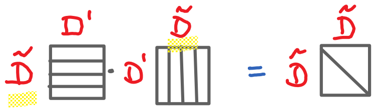
$V^\dagger$ is right isometry: $V^\dagger V =$  $= \mathbb{1}_{\tilde{D}}$ (17)

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)

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

trace is cyclic

singular values determine norm

Truncation

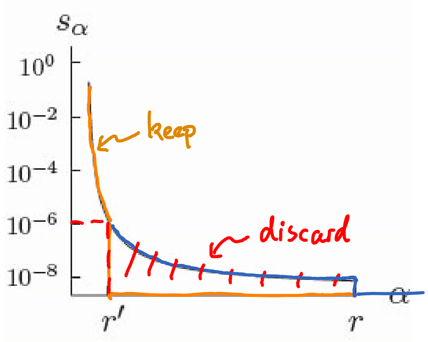
SVD can be used to approximate a rank r matrix M by a rank r' $(< r)$ matrix M' :

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!

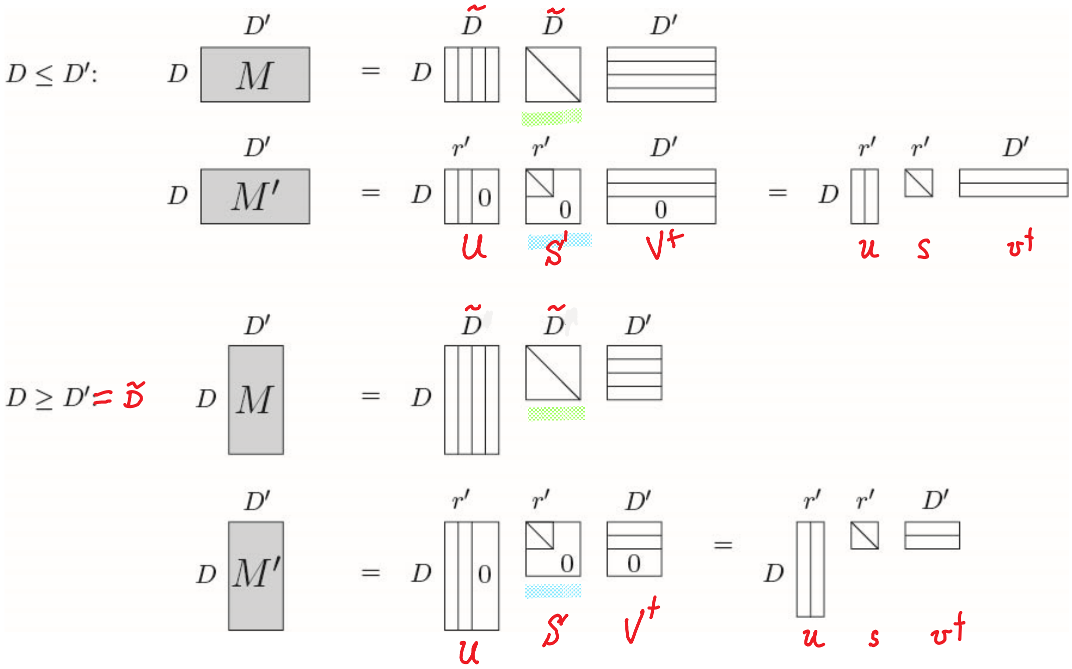
Visualization, with $r = \tilde{D}$:

$\tilde{D} =$ $D \le D'$: (27)

(28)

$D \ge D' = \tilde{D}$ (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, $M - M'$.

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

similar steps as for (8)

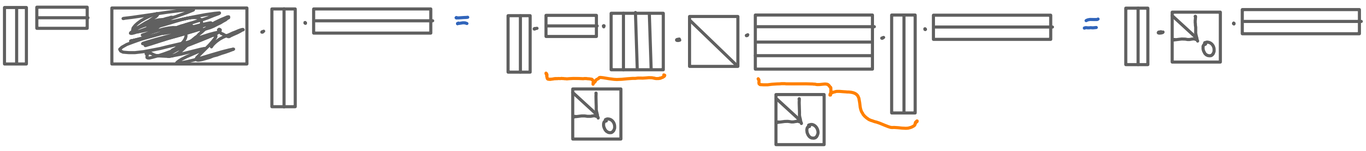
$$= \mathrm{Tr}\left(S \cdot S + S' \cdot S' - \underbrace{S' \cdot S}_{= S' \cdot S'} - \underbrace{S \cdot S'}_{= S' \cdot S'} \right) \quad (32)$$

'discarded weight'

'discarded weight'

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

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

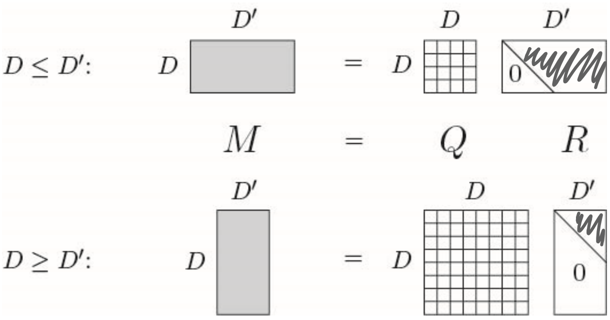
no negative eigenvalues

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

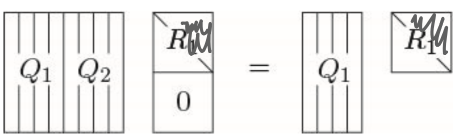
has the 'full QR decomposition'

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

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

and R a $D \times D'$ upper triangular matrix, $\quad R_{\alpha\beta} = 0$ 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. $\quad Q_1^\dagger Q_1 = \mathbb{1}$ but $Q_1 Q_1^\dagger \neq \mathbb{1} \qquad (39)$

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

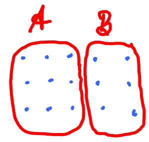
6. Schmidt decomposition [most efficient way of representing entanglement]

TNB.6

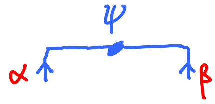
[most efficient way of representing entanglement]

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



Reduced density matrices of subsystem $\mathcal{A}$:

$$\mathrm{Tr}_{\mathcal{B}} |\beta\rangle\langle\beta'| = \delta_\beta{}^{\beta'}$$

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

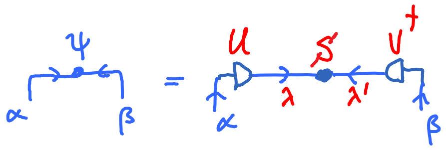
$$= |\alpha\rangle_{\mathcal{A}} (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} \, {}_{\mathcal{A}}\langle\alpha'| , \qquad \text{with} \qquad (\rho_{\mathcal{A}})^{\alpha}{}_{\alpha'} = (\psi\psi^{\dagger})^{\alpha}{}_{\alpha'} \qquad (3)$$

Singular value decomposition

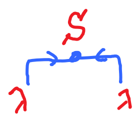
Use SVD to find bases for $\mathcal{A}$ and $\mathcal{B}$ which diagonalize density matrices:

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

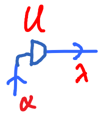
With indices: $\quad \psi^{\alpha\beta} = U^{\alpha}{}_{\lambda} \, \underbrace{S^{\lambda\lambda'}}_{\mathrm{diag}(s_1, s_2, \dots)} \, V^{\dagger}{}_{\lambda'}{}^{\beta}$ (5)



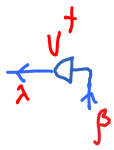
Hence $\quad |\psi\rangle = |\lambda'\rangle_{\mathcal{A}} |\lambda\rangle_{\mathcal{B}} S^{\lambda\lambda'} = \sum_{\lambda} |\lambda\rangle_{\mathcal{A}} |\lambda\rangle_{\mathcal{B}} s_{\lambda}$ (6)



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



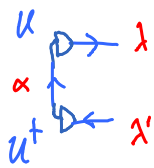
; $\quad |\lambda\rangle_{\mathcal{B}} = |\beta\rangle V^{\dagger}{}_{\lambda}{}^{\beta}$, (7)

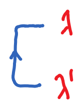


are orthonormal sets of states for $\mathcal{A}$ and $\mathcal{B}$, and can be extended to yield orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$ if needed.

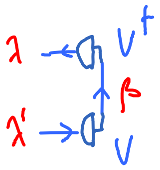
Orthonormality is guaranteed by $\quad U^{\dagger} U = \mathbb{1}$ and $V^{\dagger} V = \mathbb{1}$! (8)

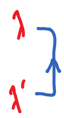
$${}_{\mathcal{A}}\langle\lambda'|\lambda\rangle_{\mathcal{A}} = \quad = U^{\dagger\lambda'}{}_{\alpha} U^{\alpha}{}_{\lambda} = \mathbb{1}^{\lambda'}{}_{\lambda} = \qquad (9)$$





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





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

In this representation, reduced density matrices are diagonal:

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

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

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

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, $S_{A|B} = \ln r$ (this proves (TNB1.13) (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:

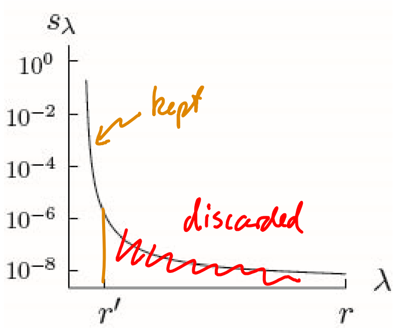
$$|\tilde{\psi}\rangle \equiv \sum_{\lambda=1}^{r'} |\lambda\rangle_A |\lambda\rangle_B s_\lambda \qquad (18)$$

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



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 $s_\lambda \left[\sum_{\lambda'=1}^{r'} (s_{\lambda'})^2 \right]^{-1/2}$ (20)

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