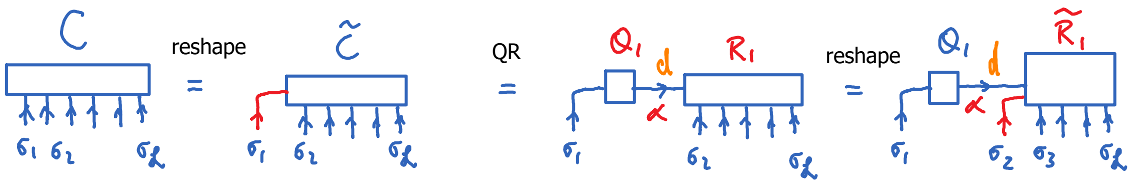
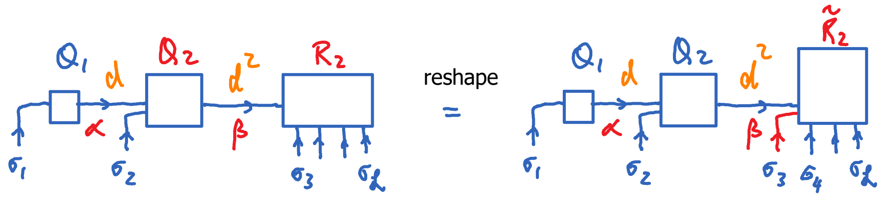
Tensor network basics III

1. Reshaping generic tensor into MPS form

A generic tensor of arbitrary rank can be expressed as an MPS through repeated matrix factorizations, using QR decomposition, $M \overset{\text{TNB-III.2}}{=} QR$, or singular value decomposition (SVD): $M \overset{\text{TNB-III.2}}{=} USV^\dagger$



(1)



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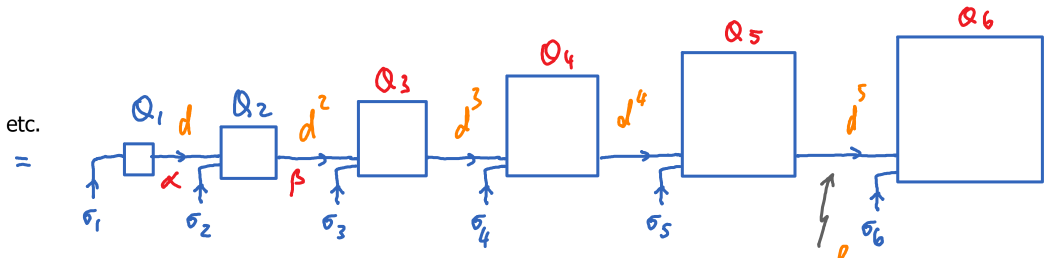


(3)

bond dimensions grow as d^ℓ

In formulas ('reshape' means regroup indices):

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

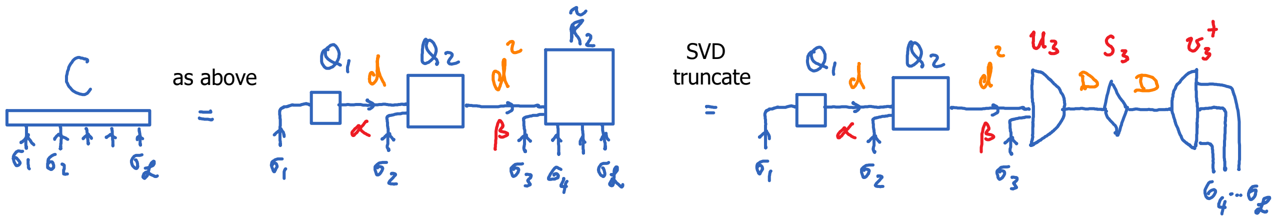
$$\overset{\text{QR}}{=} Q_1^{\sigma_1}{}_{\alpha}\, Q_2^{\alpha\sigma_2}{}_{\beta}\, R_2^{\beta,\sigma_3\cdots\sigma_\ell} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_{\alpha}\, Q_2^{\alpha\sigma_2}{}_{\beta}\, \tilde{R}_2^{\beta\sigma_3,\sigma_4\cdots\sigma_\ell} \overset{\text{etc.}}{=} \dots \qquad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

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

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:

$R \overset{\text{SVD}}{=} USV^\dagger$ (U and V are isometries, S is diagonal, with non-negative elements)

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



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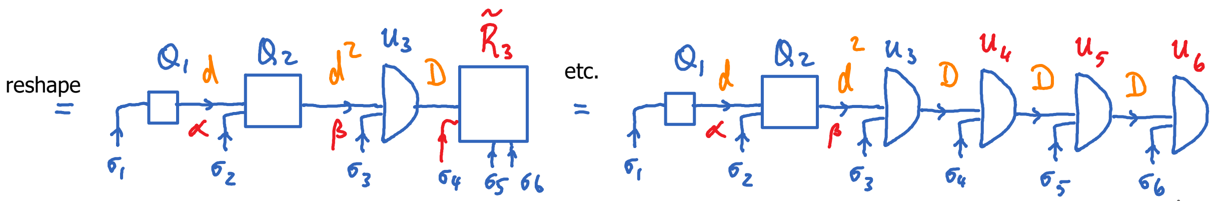


truncated representation (8)

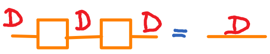
2. Unitaries and isometries (reminder)

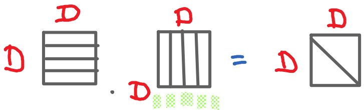
TNB-III.2

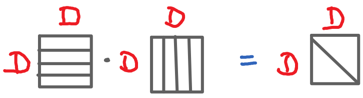
Unitaries

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

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







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 $\mathbb{C}^D$

U defines an invertible map: position j, column j; (standard basis vector in $\mathbb{C}^D$) $\quad = u_j \in \mathbb{C}^D, \quad j = 1, \dots, D$ (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 $\mathbb{C}^D$: $\vec{e}_i = (0, \dots, 0, 1, 0, \dots, 0)^T$ ← 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)

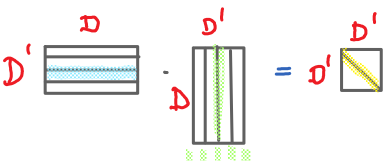
Left isometry

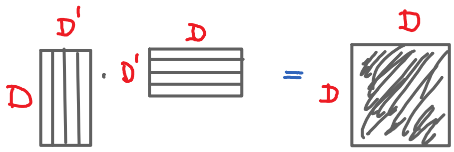
(isometry = distance-preserving map)

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

$$A^\dagger A = \mathbb{1}_{D'} \quad (6a)$$

Note: if $D > D'$ then $A A^\dagger \neq \mathbb{1}_D$ (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

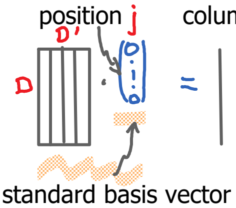
$u \quad - \quad u_l$

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 $\mathbb{C}^{*D'}$, <u>not</u> $\mathbb{C}^{*D}$]
↖ dual space of D'-dimensional row vectors

A defines an isometric map:



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

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

Formally:

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

short column vectors → long column vectors; $\vec{e}_i$: 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

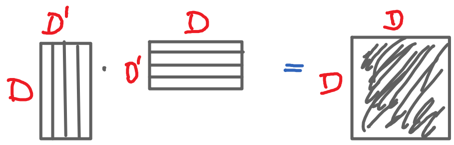
<u>Invariance of scalar product</u> (hence the name: iso-metric = equal metric):

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

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

<u>Left projector</u>

$= P = AA^\dagger =$



(11)

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

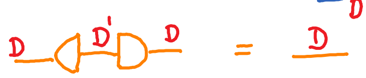
Its action leaves V_A invariant, because it leaves each its basis vectors invariant: (13)

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

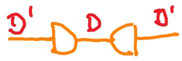
Right isometry

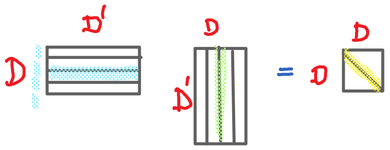
A rectangular matrix $B \in \mathrm{mat}(D, D'; \mathbb{C})$ with $D \leq D'$ is called a 'right isometry' if (14a) holds:

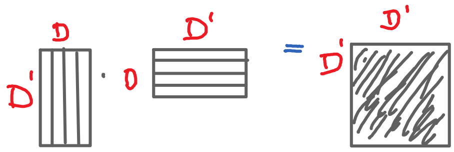
$$B B^\dagger = \mathbb{1}_D \qquad (14a)$$



Note: if $D < D'$ then $B^\dagger B \neq \mathbb{1}_{D'}$ (14b)







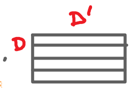
Its D row vectors, $B = \begin{pmatrix} \vec{b}^1 \\ \vec{b}^2 \\ \vdots \\ \vec{b}^D \end{pmatrix}$, are orthonormal, $\vec{b}^i \cdot \vec{b}^{\dagger}{}_j \overset{(6a)}{=} \delta^i{}_j$. (15)

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

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

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

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

short row vectors → long row vectors; $\vec{e}^j$: 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):

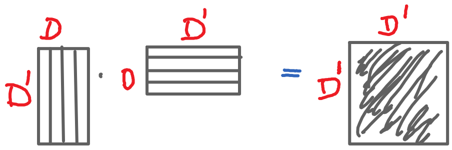
If $B : \mathbb{C}^{D*} \to \mathbb{C}^{D'*}$, $\vec{x} \mapsto \vec{y} = \vec{x} B$, then

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

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

Right projector

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



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

(14a)

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

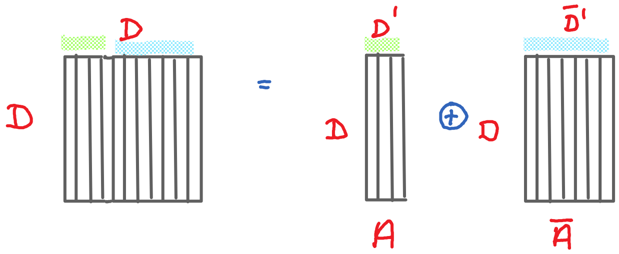
$$\vec{b}^i P \overset{(19,17b)}{=} \vec{f}^{\,i}\,\underbrace{B\,B^\dagger}_{(14a)\,=\,\mathbb{1}}B = \vec{f}^{\,i} B \overset{(17b)}{=} \vec{b}^i \quad ✓ \qquad (21)$$

Truncation of unitaries yield isometries

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

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

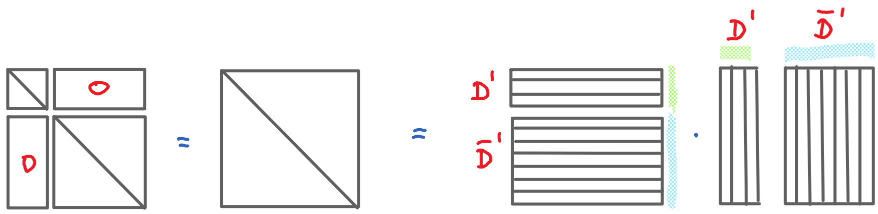
$$U = (\vec{u}_1, \vec{u}_2, \dots \vec{u}_{D'}, \vec{u}_{D'+1}, \dots \vec{u}_D) = (\vec{u}_1, \dots, \vec{u}_{D'}) \oplus (\vec{u}_{D'+1}, \dots, \vec{u}_D) =: A \oplus \bar{A} \qquad (23)$$



(24)

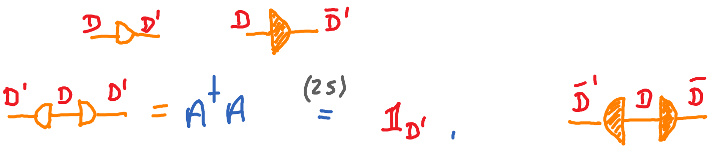
Unitarity of U implies:

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

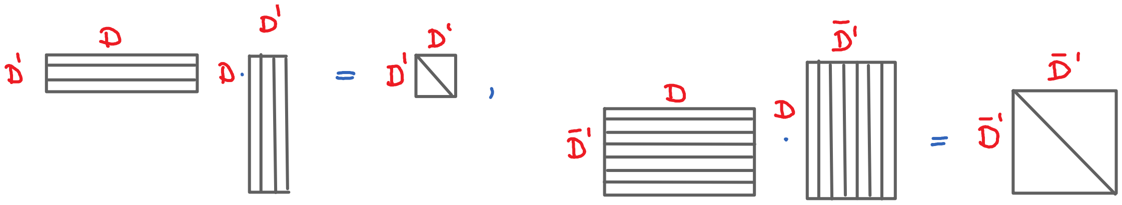


(26)

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



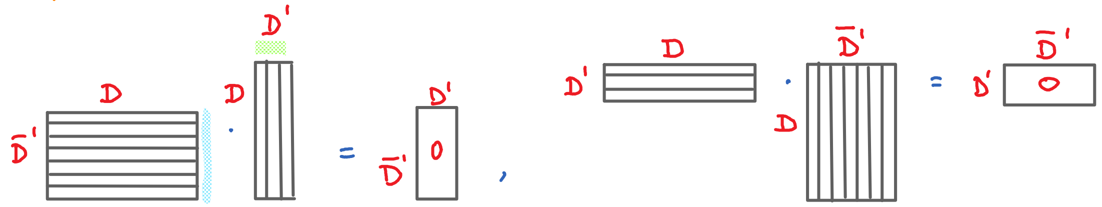
$$= A^\dagger A \overset{(25)}{=} \mathbb{1}_{D'} \,, \qquad = \bar{A}^\dagger \bar{A} \overset{(25)}{=} \mathbb{1}_{\bar{D}'} \qquad (27)$$



(28)

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

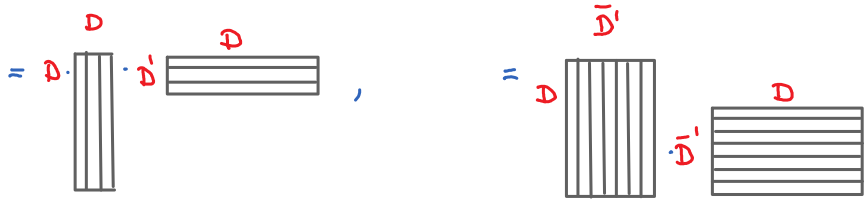
 $= \bar{A}^\dagger A \overset{(25)}{=} 0$,  $= A^\dagger \bar{A} \overset{(25)}{=} 0$ (29)



(30)

Complementary projectors

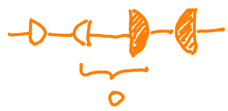
The projectors, $P = A A^\dagger =$  , $\bar{P} = \bar{A} \bar{A}^\dagger =$  (31)



are both $D \times D$ matrices,

and satisfy orthonormality relations: (32)

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

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:

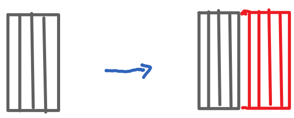
$$P : \mathbb{C}^D \to V_A = \mathrm{span}\{\vec{u}_1, \dots \vec{u}_{D'}\} =: \mathrm{span}\{\vec{a}_1, \dots, \vec{a}_{D'}\} \subsetneq \mathbb{C}^D \qquad (35)$$

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

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

3. Singular value decomposition (SVD) [Schollwoeck2011, Sec. 4] TNB-III.3

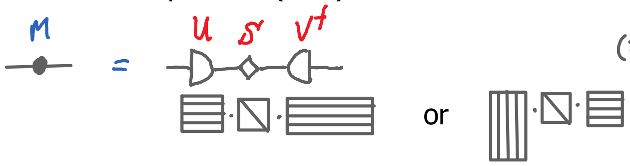
ttps://en.wikipedia.org/wiki/Singular_value_decomposition

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

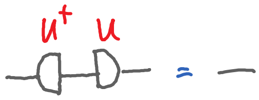
$$\boxed{M = U \cdot S \cdot V^\dagger} \quad (2)$$

$D\times D'$ $\quad D\times\tilde D$ $\quad \tilde D\times\tilde D$ $\quad \tilde D\times D'$

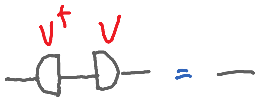


where

$U \in \mathrm{mat}(D, \tilde D; \mathbb{C})$ 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, called 'singular values' (5)

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Remarks:

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

$D\times D$: $MM^\dagger \overset{(2)}{=} (USV^\dagger)(VSU^\dagger) \overset{(4)}{=} US^2U^\dagger \overset{(3)}{\Rightarrow}$ $D\times\tilde D$: $MM^\dagger U = US^2$ (6)

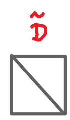
(with $V^\dagger V = \mathbb{1}$)

$D'\times D'$: $M^\dagger M \overset{(2)}{=} (VSU^\dagger)(USV^\dagger) \overset{(3)}{=} VS^2V^\dagger \overset{(4)}{\Rightarrow}$ $D'\times\tilde D$: $M^\dagger M V = VS^2$ (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: $s_1 \geq s_2 \geq \ldots \geq s_r > 0$ (9)

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

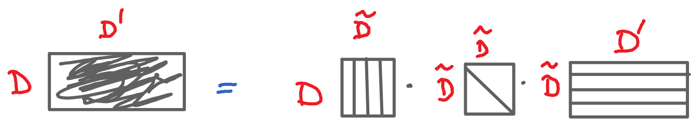
(iii) Properties of U and $V^\dagger$: $\tilde D = \min(D, D')$

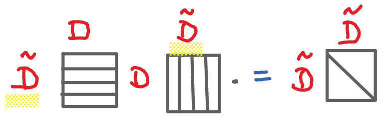
- $\dim(U) = D\times\tilde D$, $\boxed{U^\dagger U = \mathbb{1}_{\tilde D}}$, columns of U are orthonormal. (11)

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

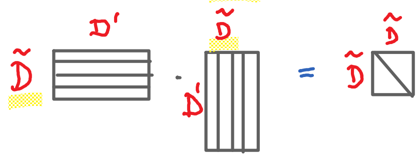
(iv) Visualization

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

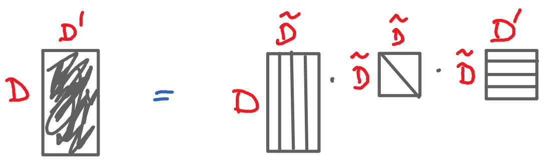
$M =$  $= U \cdot S \cdot V^\dagger$ (15)

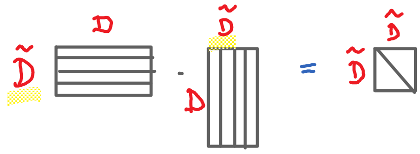
U is unitary: $U^\dagger U =$  $= \mathbb{1}_{\tilde{D}}$ (16)

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

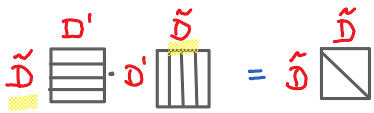
$V^\dagger$ is right isometry: $V^\dagger V =$  $= \mathbb{1}_{\tilde{D}}$ (17)

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

trace is cyclic

singular values determine norm

Truncation

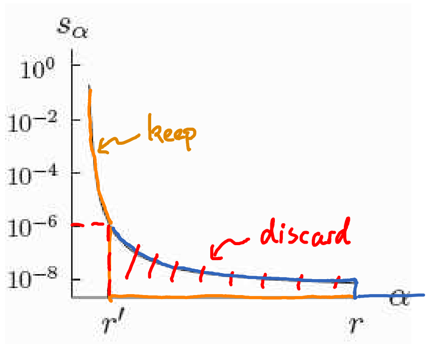
SVD can be used to approximate a rank r matrix M by a rank r' $(< r)$ matrix M' :

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

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

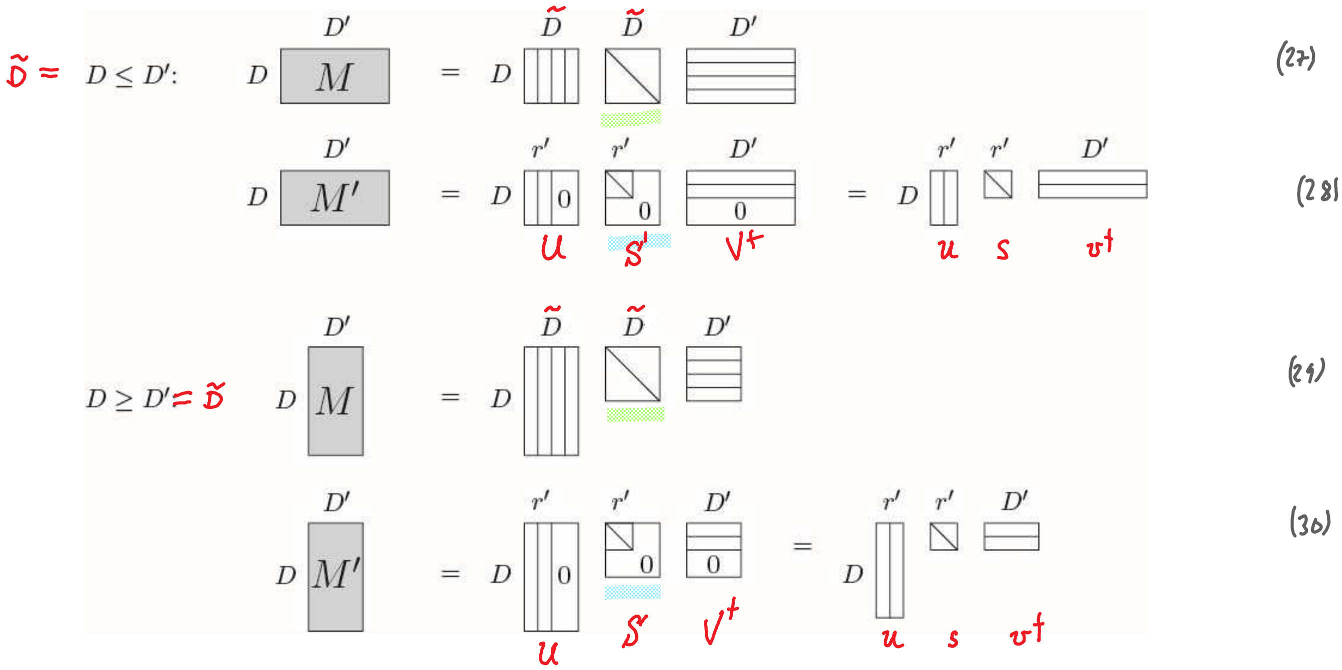
Truncate: $\boxed{M' := U S' V^\dagger}$ (25)

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 $r = \tilde{D}$:



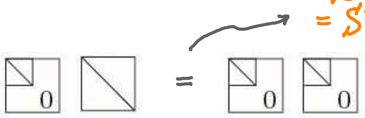
SVD truncation yields 'optimal' approximation of a rank r matrix M by a rank r' $(< r)$ matrix M',

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)

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

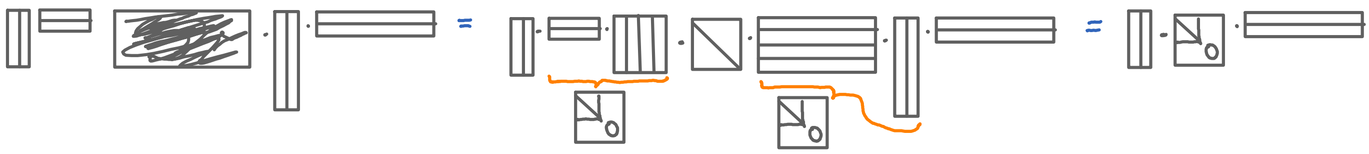


'discarded weight'

'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:

$$M = USV^\dagger = \begin{cases} (USU^\dagger)(UV^\dagger) = PW & \text{'left polar decomposition'} \\ (UV^\dagger)(VSV^\dagger) = \tilde{W}\tilde{P} & \text{'right polar decomposition'} \end{cases} \qquad (34)$$

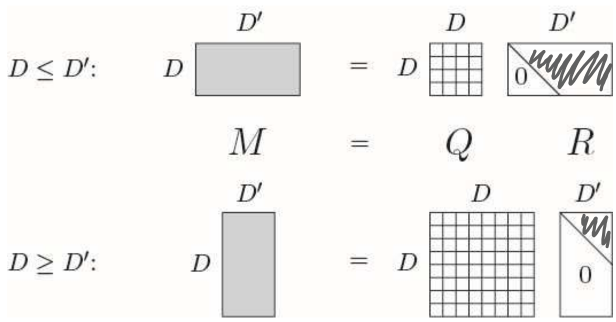
This generalizes the polar decomposition for complex numbers, $z = |z| e^{i\phi}$

QR-decomposition

If singular values are not needed,

a $D \times D'$ matrix M

has the 'full QR decomposition'



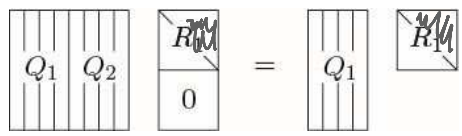
$$M = QR \qquad (35)$$

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

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

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

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



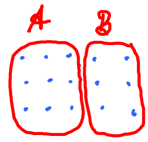
with dim(Q1) = $D \times D'$, dim(R1) = $D' \times D'$, and R1 upper triangular. $Q_1^\dagger Q_1 = \mathbb{1}$ but $Q_1 Q_1^\dagger \neq \mathbb{1}$ (39)

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

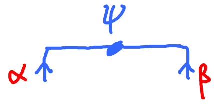
4. Schmidt decomposition

[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 $\mathcal{A} \cup \mathcal{B}$: $|\psi\rangle = |\alpha\rangle_{\mathcal{A}} |\beta\rangle_{\mathcal{B}} \psi^{\alpha\beta}$



(1)

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

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

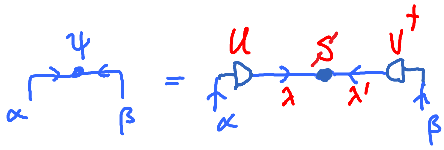
$$\hat{\rho}_{\mathcal{B}} = \mathrm{Tr}_{\mathcal{A}} |\psi\rangle\langle\psi| = |\beta\rangle_{\mathcal{B}} (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} \, {}_{\mathcal{B}}\langle\beta'| , \qquad (\rho_{\mathcal{B}})^{\beta}{}_{\beta'} = (\psi^{\dagger}\psi)_{\beta'}{}^{\beta} \qquad (3)$$

Singular value decomposition

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

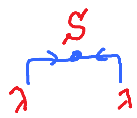
$$\psi \overset{\text{SVD}}{=} U S V^{\dagger} \qquad (4)$$

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

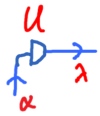
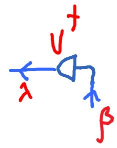


(5)

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



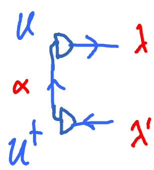
(6)

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

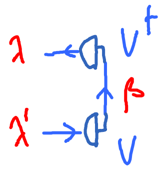
are orthonormal sets of states for $\mathcal{A}$ and $\mathcal{B}$, and can be extended to yield orthonormal bases for $\mathcal{A}$ and $\mathcal{B}$ if needed.

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

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



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



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

In this representation, reduced density matrices are diagonal:

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

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

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

Entangement 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 $|\psi\rangle = \sum_{\alpha\beta} |\alpha\rangle_A |\beta\rangle_B \psi^{\alpha\beta}$ by cheaper $|\tilde{\psi}\rangle$?

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

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

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

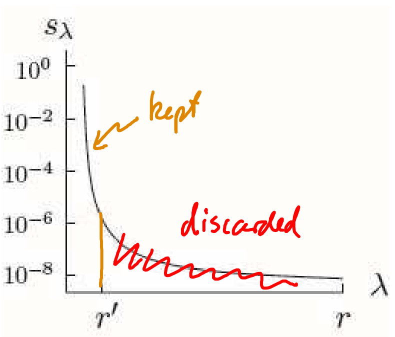
If $|\tilde{\psi}\rangle$ should be normalized, rescale, i.e. replace s_λ by $s_\lambda \left[\sum_{\lambda'=1}^{r'} (s_{\lambda'})^2 \right]^{-1/2}$ (19)

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.