

1. Overlaps and normalization $\langle \psi | \psi \rangle$

Consider overlap of 2-site MPS:

$$|\beta\rangle = |\sigma_2\rangle|\sigma_1\rangle A^{\alpha\sigma_1} B^{\alpha\sigma_2} \beta \quad (1)$$

dummy index

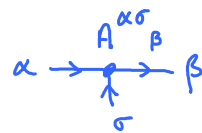
$$\langle \beta' | \beta \rangle = \overbrace{A^{\alpha'\sigma_1'}}_{\alpha'} \overbrace{B^{\alpha\sigma_2'}}_{\beta'} \langle \sigma_1' | \langle \sigma_2' | \sigma_2 \rangle \sigma_1 \rangle A^{\alpha\sigma_1} B^{\alpha\sigma_2} \beta \quad (2)$$

introduce A^{\dagger} 's: $A^{\dagger\alpha'\sigma_1'} B^{\beta'\sigma_2'\alpha'}$ (3)

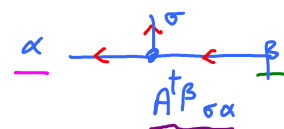
reorder A^{\dagger} 's: $B^{\beta'\sigma_2'\alpha'} A^{\dagger\alpha'\sigma_1'} A^{\alpha\sigma_1} B^{\alpha\sigma_2} \beta$ (4)

Use diagrammatic rules to keep track of contraction patterns:

Ket: $|\beta\rangle = |\sigma\rangle|\alpha\rangle A^{\alpha\sigma} \beta$ (5)



Bra: $\langle \beta' | = \langle \alpha' | \langle \sigma' | \overline{A^{\alpha\sigma}} \beta' \equiv A^{\dagger\beta'\sigma'\alpha'}$ (6)



We accommodated complex conjugation via Hermitian conjugation and index transposition:

$$A^{\dagger\beta'\sigma'\alpha'} = \overline{A^{\alpha\sigma} \beta}$$

This moves upstairs indices downstairs and vice versa, i.e. inverts all arrows in diagram.

Note that in diagram vertex, α sits left, β right, whereas on A^{\dagger} , β sits left, α right.

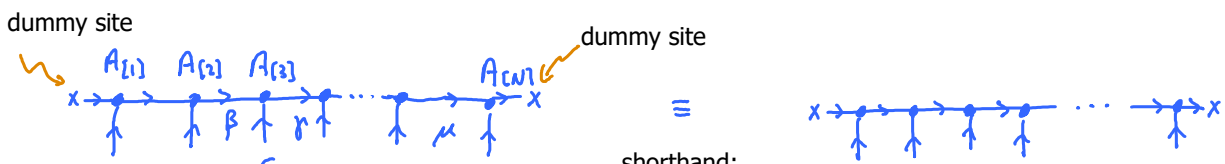
This convention may seem initially awkward, but it greatly simplifies the structure of diagrams representing overlaps.

Generalization to many-site MPS:

$$|\psi\rangle = |\sigma_N\rangle \dots |\sigma_2\rangle |\sigma_1\rangle A^{\alpha\sigma_1} A^{\alpha\sigma_2} B^{\alpha\sigma_2} \beta A^{\beta\sigma_3} \gamma \dots A^{\mu\sigma_N} \nu \quad (7)$$

dummy index

Square brackets indicate that each site has a different A matrix. We will often omit them and use the shorthand, $A^{\alpha\sigma_l} \beta \equiv A_{[l]}^{\alpha\sigma_l} \beta$, since the l on σ_l uniquely identifies the site.





Recipe for ket formula: as chain grows, attach new matrices on the right (in same order as vertices in diagram); resulting in a matrix product structure.

Bra: $\langle \sigma_1 | \langle \sigma_2 | \dots \langle \sigma_N |$

$$\langle \psi | = \langle \vec{\sigma} | A_{[1]}^{\sigma_1 \alpha} A_{[2]}^{\alpha \sigma_2 \beta} A_{[3]}^{\beta \sigma_3 \gamma} \dots A_{[N]}^{\mu \sigma_N} = A_{[N]}^{\sigma_N \mu} \dots A_{[3]}^{\delta \sigma_3 \beta} A_{[2]}^{\beta \sigma_2 \alpha} A_{[1]}^{\alpha \sigma_1} \langle \vec{\sigma} |$$

(9)

We expressed all matrices via their Hermitian conjugates by transposing indices and inverting arrows. To recover a matrix product structure, we ordered the Hermitian conjugate matrices to appear in the opposite order as the vertices in the diagram.

Recipe for bra formula: as chain grows, attach new matrices A^\dagger on the left, opposite to vertex order in diagram.

Now consider overlap between two MPS:

$$\langle \hat{\psi} | \psi \rangle =$$

Recipe: contract all physical indices!

$$= A_{[N]}^{\sigma_N \mu'} \dots A_{[3]}^{\delta \sigma_3 \beta'} \tilde{A}_{[2]}^{\beta' \sigma_2 \alpha'} \tilde{A}_{[1]}^{\alpha' \sigma_1} A_{[1]}^{\sigma_1 \alpha} A_{[2]}^{\alpha \sigma_2 \beta} A_{[3]}^{\beta \sigma_3 \gamma} \dots A_{[N]}^{\mu \sigma_N} \quad (10)$$

Exercise: derive this result algebraically from (7), (9),

If we would perform the matrix multiplication first, for fixed $\vec{\sigma}$, and then sum over $\vec{\sigma}'$, we would get d^N terms, each of which is a product of $2N$ matrices. Exponentially costly! 😞

But calculation becomes tractable if we rearrange summations:

$$\langle \tilde{\psi} | \psi \rangle = C_{[N]} \cdots C_{[2]} C_{[1]} C_{[0]} \quad (11)$$

$$= \tilde{A}_{\sigma_N \mu'}^{\dagger 1} \cdots \tilde{A}_{\sigma_2 \alpha'}^{\dagger 1} \underbrace{A_{\sigma_1 \alpha'}^{\dagger 1} \cdot A_{[1]}^{\alpha \sigma_1} A_{[2]}^{\alpha \sigma_2} \cdots A_{[N]}^{\mu \sigma_N}}_{\equiv C_{[1]}^{\alpha'} \alpha} \equiv C_{[2]}^{\beta'} \beta \cdots \equiv C_{[N]}^{\dagger 1} \quad (12)$$

Diagrammatic depiction: 'closing zipper' from left to right.

$$C_{[0]} \begin{array}{c} \xrightarrow{\alpha} \\ \uparrow \sigma_1 \\ \xleftarrow{\alpha'} \\ \downarrow \beta' \end{array} \begin{array}{c} \xrightarrow{\beta} \\ \uparrow \sigma_2 \\ \xleftarrow{\beta'} \\ \downarrow \sigma_3 \end{array} \begin{array}{c} \xrightarrow{\gamma} \\ \uparrow \sigma_3 \\ \xleftarrow{\gamma'} \\ \downarrow \sigma_4 \end{array} \cdots \begin{array}{c} \xrightarrow{x} \\ \uparrow \sigma_N \\ \xleftarrow{x'} \\ \downarrow \sigma_N \end{array} = C_{[1]} \begin{array}{c} \xrightarrow{\alpha} \\ \uparrow \sigma_2 \\ \xleftarrow{\alpha'} \\ \downarrow \beta' \end{array} \begin{array}{c} \xrightarrow{\beta} \\ \uparrow \sigma_3 \\ \xleftarrow{\beta'} \\ \downarrow \sigma_4 \end{array} \cdots \begin{array}{c} \xrightarrow{x} \\ \uparrow \sigma_N \\ \xleftarrow{x'} \\ \downarrow \sigma_N \end{array} = C_{[2]} \begin{array}{c} \xrightarrow{\beta} \\ \uparrow \sigma_3 \\ \xleftarrow{\beta'} \\ \downarrow \sigma_4 \end{array} \cdots \begin{array}{c} \xrightarrow{x} \\ \uparrow \sigma_N \\ \xleftarrow{x'} \\ \downarrow \sigma_N \end{array} = C_{[N]} \quad (13)$$

The set of two-leg tensors $C_{[l]}$ can be computed iteratively:

Initialization: $C_{[0]} \begin{array}{c} \xrightarrow{x} \\ \uparrow \\ \xleftarrow{x} \\ \downarrow \end{array} = \left[\begin{array}{c} \xrightarrow{x} \\ \uparrow \\ \xleftarrow{x} \\ \downarrow \end{array} \right] \quad (identity) \quad C_{[0]}^{\dagger 1} = 1 \quad (14)$

Iteration step: $C_{[l]} \begin{array}{c} \xrightarrow{\lambda} \\ \uparrow \sigma_l \\ \xleftarrow{\lambda'} \\ \downarrow \gamma' \end{array} = C_{[l-1]} \begin{array}{c} \xrightarrow{\gamma} \\ \uparrow \sigma_{l-1} \\ \xleftarrow{\gamma'} \\ \downarrow \lambda' \end{array} \quad C_{[l]}^{\lambda' \lambda} = \tilde{A}_{\sigma_l \gamma'}^{\dagger \lambda'} C_{[l-1]}^{\gamma' \lambda} A^{\lambda \sigma_l} \quad (15)$

Final answer: $\langle \tilde{\psi} | \psi \rangle = C_{[N]}^{\dagger 1} \quad (16)$

Cost estimate (if all A's are $D \times D$):

One iteration: $\underbrace{D^2 d}_{\text{fixed}} \cdot \underbrace{D}_{\text{sum}} + \underbrace{D^2}_{\text{fixed}} \cdot \underbrace{dD}_{\text{sum}} \quad \begin{array}{c} \xrightarrow{\lambda} \\ \uparrow \sigma \\ \xleftarrow{\lambda'} \\ \downarrow \gamma' \end{array} = \begin{array}{c} \xrightarrow{\lambda} \\ \uparrow \sigma \\ \xleftarrow{\lambda'} \\ \downarrow \gamma' \end{array} = \left[\begin{array}{c} \xrightarrow{\lambda} \\ \uparrow \sigma \\ \xleftarrow{\lambda'} \\ \downarrow \gamma' \end{array} \right] \quad (17)$

Total cost: $\sim D^3 d \cdot N \quad (18)$

Remark: a similar iteration scheme can be used to 'close zipper from right to left':

$$D_{[N+1]} = D_{[N-1]} = \dots = D_{[1]} \quad (19)$$

Initialization: $D_{[N+1]} = \begin{matrix} \lambda \\ \downarrow \\ \uparrow \\ \lambda' \end{matrix}$ (identity), Iteration step: $D_{[l]} = \begin{matrix} \lambda \\ \downarrow \\ \uparrow \\ \lambda' \end{matrix} = \begin{matrix} \lambda \\ \downarrow \\ \uparrow \\ \lambda' \end{matrix} \begin{matrix} \sigma \\ \leftarrow \\ \rightarrow \\ \sigma \end{matrix} D_{[l+1]}$ (20)

Normalization $\langle \psi | \psi \rangle = ?$

Use above scheme, with $\tilde{A} = A$

Left-normalization

A 3-leg tensor $A^{\alpha\sigma}_{\beta}$ is called 'left-normalized' if it satisfies

$A^{\dagger} A = \mathbb{1}$

 . Explicitly: $(A^{\dagger} A)^{\beta'}_{\beta} = A^{\dagger \beta'}_{\sigma \alpha} A^{\alpha \sigma}_{\beta} = \mathbb{1}^{\beta'}_{\beta}$ (21)

Graphical notation for left-normalization: draw 'left-pointing diagonals' at vertices

$$\begin{matrix} \alpha \\ \rightarrow \\ \leftarrow \\ \alpha' \end{matrix} \begin{matrix} A \\ \downarrow \\ \uparrow \\ A^{\dagger} \end{matrix} \begin{matrix} \beta \\ \leftarrow \\ \rightarrow \\ \beta' \end{matrix} = \begin{matrix} \beta \\ \leftarrow \\ \rightarrow \\ \beta' \end{matrix} \quad \text{identity matrix} \quad (22)$$

When all A's are left-normalized, closing the zipper left-to-right is easy, since all $C_{[l]}$ reduce to identity matrices:

$$C_{[0]} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix}, \quad C_{[1]}^{\alpha'}_{\alpha} = \begin{matrix} \alpha' \\ \leftarrow \\ \rightarrow \\ \alpha \end{matrix} = \begin{matrix} \alpha \\ \leftarrow \\ \rightarrow \\ \alpha' \end{matrix}, \quad C_{[l]}^{\lambda} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} = C_{[l-1]}^{\lambda} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} \quad (23)$$

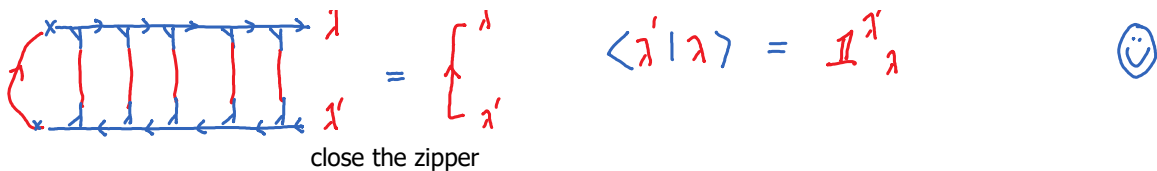
Hence:

$$\langle \psi | \psi \rangle = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} = \begin{matrix} \lambda \\ \leftarrow \\ \rightarrow \\ \lambda' \end{matrix} = \mathbb{1} \quad \text{😊} \quad (24)$$

When all matrices of a MPS are left-normalized, the matrices for site 1 to any site $l = 1, \dots, N$ define an orthonormal state space:

$$|\lambda\rangle = |\sigma_l\rangle [A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_l}]^{\lambda}$$

$$\langle \lambda' | \lambda \rangle = \mathbb{1}^{\lambda'}_{\lambda} \quad \text{😊}$$



Right-normalization

So far we have viewed an MPS as being built up from left to right, hence used right-pointing arrows on ket diagram. Sometimes it is useful to build it up from right to left, running left-pointing arrows.

Building blocks:

$$|\alpha\rangle = |\sigma_N\rangle B_{\alpha}^{\sigma_N} \quad (25)$$

$$|\beta\rangle = |\sigma_N\rangle |\sigma_{N-1}\rangle B_{\beta}^{\sigma_{N-1} \alpha} B_{\alpha}^{\sigma_N} \quad (26)$$

left-to-right index order as in diagram

$$\langle \alpha | = B_{\sigma_N}^{\dagger \alpha} \langle \sigma_N | \equiv \bar{B}_{\alpha}^{\sigma_N} \quad (27)$$

$$\langle \beta | = B_{\sigma_N}^{\dagger \alpha} B_{\alpha \sigma_{N-1}}^{\dagger \beta} \langle \sigma_{N-1} | \langle \sigma_N | \quad (28)$$

Iterating this, we obtain kets and bras of the form

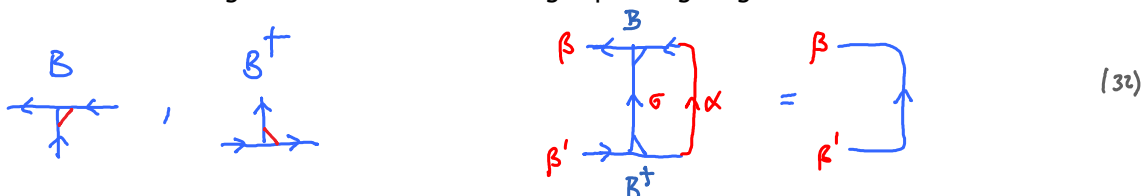
$$|\psi\rangle = |\sigma_N\rangle |\sigma_{N-1}\rangle \dots |\sigma_1\rangle B_{\sigma_1}^{\sigma_1 \lambda} \dots B_{\beta}^{\sigma_{N-1} \alpha} B_{\alpha}^{\sigma_N} \quad (29)$$

$$\langle \psi | = B_{\sigma_N}^{\dagger \alpha} B_{\alpha \sigma_{N-1}}^{\dagger \beta} \dots B_{\lambda \sigma_1}^{\dagger} \langle \sigma_1 | \dots \langle \sigma_{N-1} | \langle \sigma_N | \quad (30)$$

A three-leg tensor $B_{\beta}^{\sigma \alpha}$ is called right-normalized if it satisfies

$$B B^{\dagger} = \mathbb{1}. \quad \text{Explicitly: } (B B^{\dagger})_{\beta}^{\beta'} = B_{\beta}^{\sigma \alpha} B_{\alpha \sigma}^{\dagger \beta'} = \mathbb{1}_{\beta}^{\beta'} \quad (31)$$

Graphical notation for right-normalization: draw 'right-pointing diagonals' at vertices





When all B's are right-normalized, closing the zipper right-to-left is easy:

$$\langle \psi | \psi \rangle = \begin{array}{c} x \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ x \end{array} = \begin{array}{c} x \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ x \end{array} = \begin{array}{c} x \\ \text{---} \\ \text{---} \\ \text{---} \\ x \end{array} = \begin{array}{c} x \\ \text{---} \\ x \end{array} = 1 \quad (33)$$

When all matrices of a MPS are right-normalized, the matrices for site N to any site $\ell = 1, \dots, N$ define an orthonormal state space:

$$|\lambda\rangle = |\vec{\sigma}_\ell\rangle [B^{\sigma_\ell} B^{\sigma_{\ell+1}} \dots B^{\sigma_N}]_{\lambda'}'$$

$$\langle \lambda' | \lambda \rangle = \mathbb{I}^{\lambda'}_{\lambda} \quad \text{close the zipper} \quad \text{☺}$$

Conclusion: MPS built purely from left-normalized A 's or purely from right-normalized B 's are automatically normalized to 1. Shorter MPSs built on subchains automatically define orthonormal state spaces.

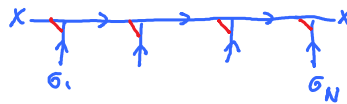


Any matrix product can be expressed through different matrices without changing the product:

$$M M' = \underbrace{(M U)}_{\tilde{M}} \underbrace{(U^{-1} M')}_{\tilde{M}'} = \tilde{M} \tilde{M}' \quad \text{'gauge freedom'}$$

Gauge freedom can be exploited to 'reshape' MPSs into particularly convenient, 'canonical' forms:

Left-canonical (lc-) MPS:

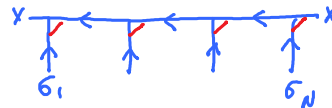


$$|\psi\rangle = |\vec{\sigma}\rangle_N (A^{\sigma_1} \dots A^{\sigma_N})$$

$$A^\dagger A = \mathbb{1}$$

$$\begin{array}{c} \rightarrow \\ \left[\begin{array}{c} \rightarrow \\ \left[\begin{array}{c} \rightarrow \\ \left[\begin{array}{c} \rightarrow \\ \rightarrow \end{array} \right] \end{array} \right] \end{array} \right] \end{array} = \left[\begin{array}{c} \rightarrow \\ \rightarrow \end{array} \right] \quad (1)$$

Right-canonical (rc-) MPS:

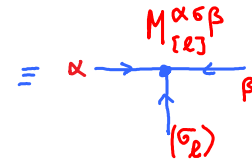
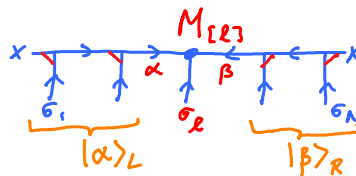


$$|\psi\rangle = |\vec{\sigma}\rangle_N (B^{\sigma_1} \dots B^{\sigma_N})$$

$$B B^\dagger = \mathbb{1}$$

$$\begin{array}{c} \left[\begin{array}{c} \left[\begin{array}{c} \left[\begin{array}{c} \left[\begin{array}{c} \leftarrow \\ \leftarrow \end{array} \right] \end{array} \right] \end{array} \right] \end{array} \right] \end{array} = \left[\begin{array}{c} \leftarrow \\ \leftarrow \end{array} \right] \quad (2)$$

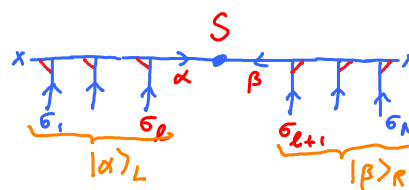
Site-canonical (sc-) MPS:



(3)

$$|\psi\rangle = |\vec{\sigma}\rangle_N (A^{\sigma_1} \dots A^{\sigma_{l-1}} M_{[l][l]}^{\sigma_l} B^{\sigma_{l+1}} \dots B^{\sigma_N}) = |\beta\rangle_R |\sigma_l\rangle |\alpha\rangle_L M^{\alpha \sigma_l \beta}$$

Bond-canonical (bc-) (or mixed) MPS:



(4)

$$|\psi\rangle = |\vec{\sigma}\rangle_N (A^{\sigma_1} \dots A^{\sigma_l}) \sum_{\alpha \beta} S_{[l][l]}^{\alpha \beta} (B^{\sigma_{l+1}} \dots B^{\sigma_N}) = \sum_{\alpha \beta} |\alpha\rangle_R S_{[l][l]}^{\alpha \beta} |\beta\rangle_L$$

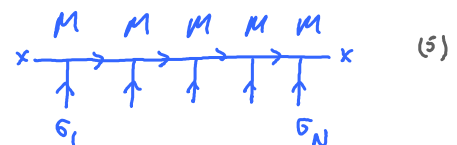
\uparrow can be chosen diagonal

How can we bring an arbitrary MPS into one of these forms?

Transforming to left-normalized form

Given:

$$|\psi\rangle = |\vec{\sigma}\rangle_N (M^{\sigma_1} \dots M^{\sigma_N})$$

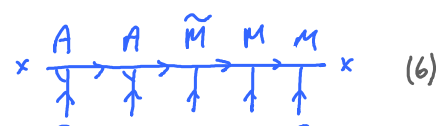


[or with index:

$$|S_N\rangle = X \rightarrow \rightarrow \rightarrow \rightarrow S_N \left. \right]$$

Goal : left-normalize

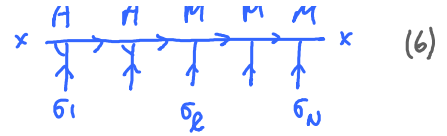
$$M^{\sigma_1} \quad \text{to} \quad M^{\sigma_{l-1}}$$



(6)

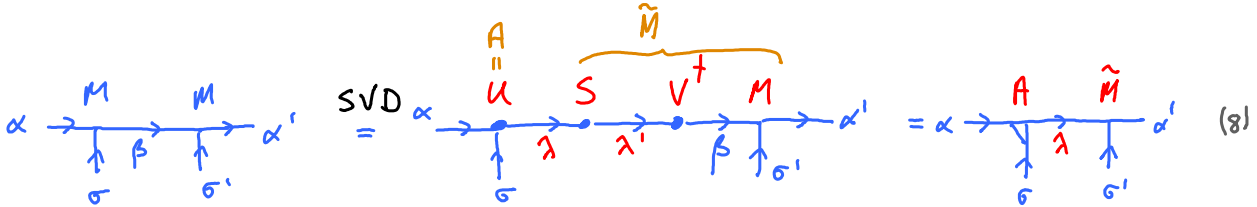
Goal : left-normalize

$$M^{\sigma_1} \text{ to } M^{\sigma_{L-1}}$$



Strategy: take a pair of adjacent tensors, MM' , and use SVD,

$$MM' = USV^T M' \equiv A \tilde{M}, \quad \text{with } A = U, \quad \tilde{M} = SV^T M' \quad (7)$$



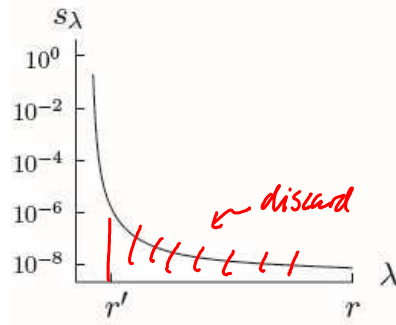
$$M^{\alpha\sigma}{}_{\beta} M^{\beta\sigma'}{}_{\alpha'} = \left(U^{\alpha\sigma}{}_{\lambda} \right) \left(\lambda \right) \left(S \lambda' V^{\lambda'\beta}{}_{\beta} M^{\beta\sigma'}{}_{\alpha'} \right) = A^{\alpha\sigma}{}_{\lambda} \tilde{M}^{\lambda\sigma'}{}_{\alpha'} \quad (9)$$

The property $U^T U = \mathbb{1}$ ensures left-normalization: $A^T A = \mathbb{1}$ (10)

Truncation, if desired, can be performed by discarding some of

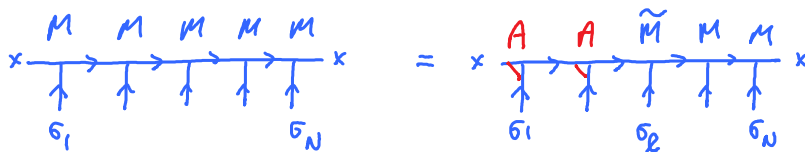
The smallest singular values,

$$\sum_{\lambda=1}^r \rightarrow \sum_{\lambda=1}^{r'} \quad (\text{but (10) remains valid!})$$



Note: instead of SVD, we could also use QR (cheaper!)

By iterating, starting from $M^{\sigma_1} M^{\sigma_2}$, we left-normalize M^{σ_1} to $M^{\sigma_{L-1}}$.



To left-normalize the entire MPS, choose $l = N$.

As last step, left-normalize last site using SVD on final \tilde{M} :

$$\tilde{M}^{\lambda\sigma_N}{}_{\beta} = \underbrace{U^{\lambda\sigma_N}{}_{\lambda'}}_{A^{\lambda\sigma_N}{}_{\lambda'}} \underbrace{S^{\lambda'\beta}{}_{\beta}}_{s_i} \underbrace{V^{\lambda'\beta}{}_{\beta}}_{1} \quad \lambda \rightarrow \tilde{M} \rightarrow \lambda \frac{U S V^T}{\sigma_N} \rightarrow \lambda \frac{A^{\sigma_N} s_i}{\sigma_N} \quad (11)$$

diamond indicates single number

lc-form: $| \psi \rangle = | \vec{\sigma} \rangle_N (A^{\sigma_1} \dots A^{\sigma_N}) s_i$

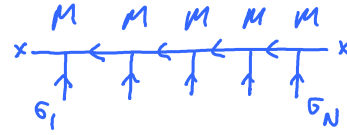
diamond indicates single number

lc-form: $|\psi\rangle = |\vec{\sigma}\rangle_N (A^{\sigma_1} \dots A^{\sigma_N}) s_1$

The final singular value, s_1 , determines normalization: $\langle\psi|\psi\rangle = |s_1|^2$. (12)

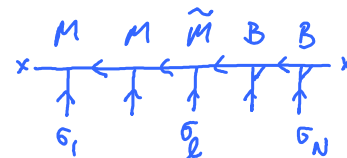
Transforming to right-normalized form

Given: $|\psi\rangle = |\vec{\sigma}\rangle_N (M^{\sigma_1} \dots M^{\sigma_N})$



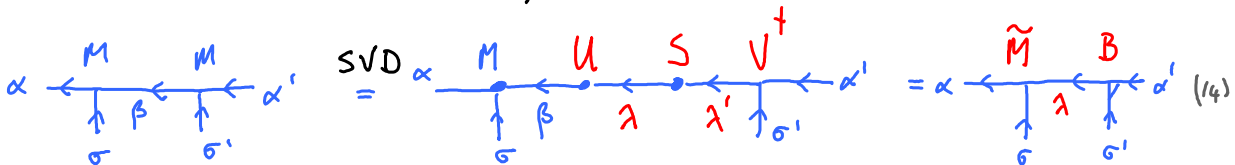
[or with index: $|s_1\rangle = s_1 \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow x$]

Goal : right-normalize M^{σ_N} to $M^{\sigma_{l+1}}$



Strategy: take a pair of adjacent tensors, MM' , and use SVD:

$$MM' = M U S U^\dagger = \tilde{M} B, \text{ with } \tilde{M} = M U S, B = U^\dagger. \quad (13)$$



$$M_{\alpha}^{\sigma\beta} M_{\beta}^{\sigma'\alpha'} = (M_{\alpha}^{\sigma\beta} U_{\beta}^{\lambda} S_{\lambda}^{\lambda'}) (U_{\lambda'}^{\sigma'\alpha'}) = \tilde{M}_{\alpha}^{\sigma\lambda} B_{\lambda'}^{\sigma'\alpha'} \quad (15)$$

Here, $U^\dagger U = \mathbf{1}$ ensures right-normalization: $B B^\dagger = \mathbf{1}$. (16)

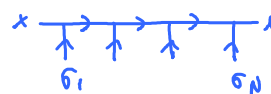
Starting form $M^{\sigma_{N-1}} M^{\sigma_N}$, move leftward up to $M^{\sigma_l} M^{\sigma_{l+1}}$.

To right-normalize entire chain, choose l and at last site, $l = 1$

$$\tilde{M}_1^{\sigma_1 \lambda} = \underbrace{U_1^{\lambda'}}_{=1} \underbrace{S_1^{\lambda'}}_{s_1} \underbrace{V_1^{\dagger \sigma_1 \lambda}}_{B_1^{\sigma_1 \lambda}} \cdot s_1 \text{ determines normalization.} \quad (17)$$

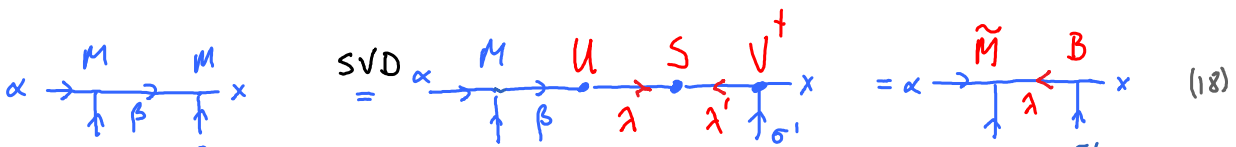
Exercise

(a) Right-normalize a state with right-pointing arrows!



Hint: start at $M^{\sigma_{N-1}} M^{\sigma_N}$

and note the up \leftrightarrow down changes in index placement.



$$\begin{aligned}
 \alpha \xrightarrow{\sigma_{N-1}} M \xrightarrow{\sigma_N} x & \stackrel{\text{SVD}}{=} \alpha \xrightarrow{\sigma} U \xrightarrow{\lambda} S \xrightarrow{\lambda'} V \xrightarrow{\sigma'} x = \alpha \xrightarrow{\sigma} \lambda \xrightarrow{\sigma'} x \quad (18) \\
 M^{\alpha\sigma} M^{\beta\sigma'} & = \left(M^{\alpha\sigma} U^{\beta\lambda} S^{\lambda\lambda'} \right) \left(V^{\lambda'\sigma'} \right) = \tilde{M}^{\alpha\sigma\lambda} B_{\lambda}^{\sigma'} \quad (19)
 \end{aligned}$$

both indices upstairs!

(b) Left-normalize a state with left-pointing arrows!



Hint: start at $M^{\sigma_1} M^{\sigma_2}$:

$$\begin{aligned}
 x \xrightarrow{\sigma_1} M \xrightarrow{\alpha} M \xrightarrow{\sigma_2} \beta & = x \xrightarrow{\sigma_1} U \xrightarrow{\lambda} S \xrightarrow{\lambda'} V^{\dagger} \xrightarrow{\alpha} M \xrightarrow{\sigma_2} \beta = x \xrightarrow{\sigma_1} A \xrightarrow{\lambda} \tilde{M} \xrightarrow{\sigma_2} \beta \quad (20) \\
 M^{\sigma_1\alpha} M^{\sigma_2\beta} & = \left(U^{\sigma_1\lambda} \right) \left(S^{\lambda\lambda'} V^{\lambda'\alpha} M^{\sigma_2\beta} \right) = A^{\sigma_1\lambda} \tilde{M}^{\lambda\sigma_2\beta} \quad (21)
 \end{aligned}$$

both indices upstairs!

Transforming to site-canonical form

$$\begin{aligned}
 x \xrightarrow{\sigma_1} M \xrightarrow{\sigma_2} M \xrightarrow{\sigma_3} M \xrightarrow{\sigma_4} M \xrightarrow{\sigma_5} x & = x \xrightarrow{\sigma_1} A \xrightarrow{\sigma_2} \tilde{M} \xrightarrow{\sigma_3} M \xrightarrow{\sigma_4} M \xrightarrow{\sigma_5} x = x \xrightarrow{\sigma_1} A \xrightarrow{\sigma_2} \tilde{M} \xrightarrow{\sigma_3} B \xrightarrow{\sigma_4} B \xrightarrow{\sigma_5} x = \tilde{M}^{\alpha\sigma_2\beta} \\
 & \quad \underbrace{\hspace{10em}}_{|\alpha\rangle_L} \quad \underbrace{\hspace{10em}}_{|\beta\rangle_R} \quad \sigma_2
 \end{aligned} \quad (22)$$

Left-normalize sites 1 to $l-1$, starting from site l .

Then right-normalize sites N to $l+1$, starting from site N .

Result:

$$|\psi\rangle = \underbrace{|\sigma_N\rangle \dots |\sigma_{l+1}\rangle}_{|\beta\rangle_R} \left(B^{\sigma_{l+1}} \dots B^{\sigma_N} \right)^{\beta} |\sigma_l\rangle |\sigma_{l-1}\rangle \dots |\sigma_1\rangle \underbrace{\left(A^{\sigma_1} \dots A^{\sigma_{l-1}} \right)^{\alpha}}_{|\alpha\rangle_L} \tilde{M}^{\alpha\sigma_l\beta} \quad (23)$$

$$= |\beta\rangle_R |\sigma_l\rangle |\alpha\rangle_L \tilde{M}^{\alpha\sigma_l\beta} \quad (24)$$

The states $|\alpha, \sigma_l, \beta\rangle \equiv |\beta\rangle_R |\sigma_l\rangle |\alpha\rangle_L$ form an orthonormal set:

$$\langle \alpha', \sigma'_l, \beta' | \alpha, \sigma_l, \beta \rangle = \delta_{\alpha'}^{\alpha} \delta_{\sigma'_l}^{\sigma_l} \delta_{\beta'}^{\beta} \quad (25)$$

(Exercise: verify this, using $A^{\dagger}A = \mathbb{1}$ and $BB^{\dagger} = \mathbb{1}$.)

This is 'local site basis' for site l . Its dimension $D_{\alpha} \cdot d \cdot D_{\beta}$ is usually $\lll d^N$ of full Hilbert space.

Transforming to bond-canonical form

$$\dots + \dots + \dots$$

Transforming to bond-canonical form

Start from (e.g.) sc-form, use SVD for $\bar{M} = USV^\dagger$, combine ① V^\dagger with neighboring B , or ② U with neighboring A .

$$\begin{array}{c}
 A \ A \ \bar{M} \ B \ B \\
 \times \rightarrow \rightarrow \rightarrow \leftarrow \leftarrow \leftarrow \times \\
 \downarrow \downarrow \downarrow \downarrow \downarrow \\
 \alpha \ \beta \\
 \mathcal{G}_l
 \end{array}
 \stackrel{\textcircled{1}}{=}
 \begin{array}{c}
 A \ A \ A \ S \ \tilde{B} \ B \\
 \times \rightarrow \rightarrow \rightarrow \leftarrow \leftarrow \leftarrow \times \\
 \downarrow \downarrow \downarrow \downarrow \downarrow \\
 \alpha \ \lambda \ \lambda' \\
 \mathcal{G}_l
 \end{array}
 =
 \underbrace{|\lambda'\rangle_R}_{\text{involves sites } l+1 \text{ to } N} \cdot \underbrace{|\lambda\rangle_L}_{\text{involves sites } 1 \text{ to } l} S^{\lambda\lambda'} \quad (26)$$

$$\bar{M} = USV^\dagger \quad A = U, \ \tilde{B} = V^\dagger B \quad (\text{Exercise: add indices!}) \quad (27)$$

The states $|\lambda, \lambda'\rangle \equiv |\lambda\rangle_R |\lambda'\rangle_L$ form an orthonormal set.

$$\langle \bar{\lambda}, \bar{\lambda}' | \lambda, \lambda' \rangle = \delta_{\bar{\lambda}}^{\lambda} \delta_{\bar{\lambda}'}^{\lambda'} \quad (28)$$

This is called the 'local bond basis for bond l ' (from site l to $l+1$). It has dimension $\tau \cdot \tau$ (τ = dimension of singular matrix S).

$$\begin{array}{c}
 A \ A \ \bar{M} \ B \ B \\
 \times \rightarrow \rightarrow \rightarrow \leftarrow \leftarrow \leftarrow \times \\
 \downarrow \downarrow \downarrow \downarrow \downarrow \\
 \alpha \ \beta \\
 \mathcal{G}_l
 \end{array}
 \stackrel{\textcircled{2}}{=}
 \begin{array}{c}
 A \ \tilde{A} \ S \ B \ B \ B \\
 \times \rightarrow \rightarrow \rightarrow \leftarrow \leftarrow \leftarrow \times \\
 \downarrow \downarrow \downarrow \downarrow \downarrow \\
 \lambda \ \lambda' \ \beta \\
 \mathcal{G}_l
 \end{array}
 =
 \underbrace{|\lambda'\rangle_R}_{\text{involves sites } l \text{ to } N} \cdot \underbrace{|\lambda\rangle_L}_{\text{involves sites } 1 \text{ to } l-1} S^{\lambda\lambda'} \quad (29)$$

$$\bar{M} = USV^\dagger \quad \tilde{A} = AU, \ B = V^\dagger \quad (\text{Exercise: add indices!}) \quad (30)$$

$|\lambda, \lambda'\rangle \equiv |\lambda'\rangle_R |\lambda\rangle_L$ form 'local bond basis' for bond $l-1$ (from site $l-1$ to l).