MPS.3 Left- and right-normalized MPS

Computation of normalization and matrix elements of local operators is simpler if the MPS is built from tensors with special normalization properties, called 'left-normalized' or 'right-normalized' tensors.

Left-normalization

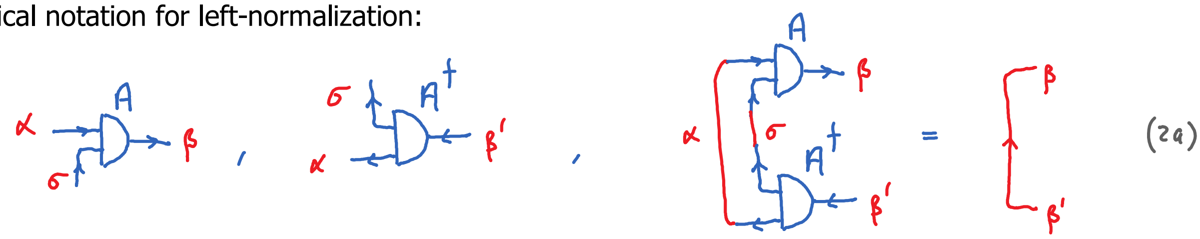
A 3-leg tensor $A^{\alpha\sigma}{}_{\beta}$ is called 'left-normalized' if it is a left isometry, i.e. if it satisfies

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

Such an A defines an 'isometry' from space labeled by its left indices to space labeled by its right indices.

distance-preserving map (in index-free notation: if $y = Ax$, then $y^\dagger y = x^\dagger A^\dagger A x = x^\dagger x$)

Graphical notation for left-normalization:

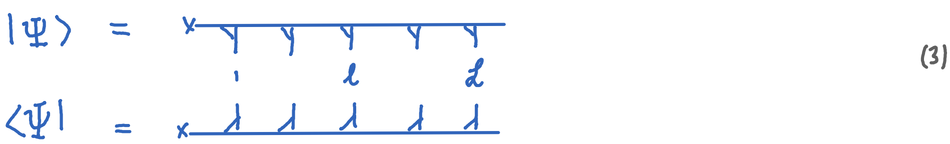


More compact notation: draw 'left-facing diagonals' at vertices

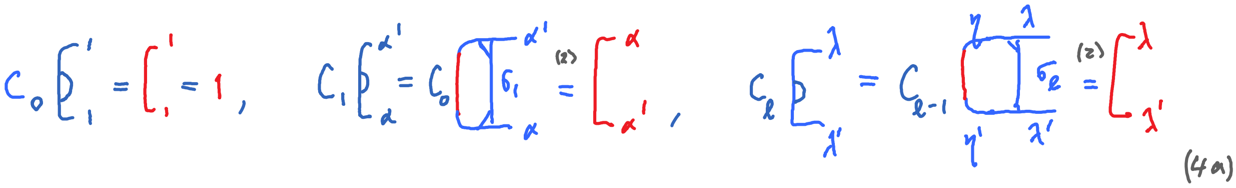
identity matrix

The right-angled triangle contains complete information about all arrows attached to it:
for A , incoming arrows to sharp angles, outgoing arrow from right angle,
for $A^\dagger$, outgoing arrows from sharp angles, incoming to from right angle:
Hence, there is no need to draw arrows explicitly when using $\top$, $\perp$!

Consider a 'left-normalized MPS', i.e. one constructed purely from left isometries:



Then, closing the zipper left-to-right is easy, since all C_ℓ reduce to identity matrices:



We suppress arrows for C, too, since they can be reconstructed from arrows of constitutent As.

Hence:

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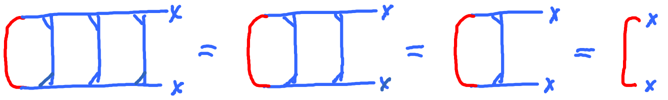
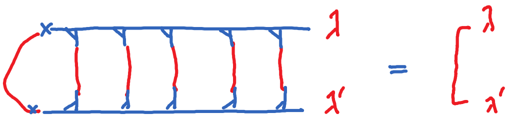
Hence:

$\langle\Psi|\Psi\rangle =$  $= 1$ (4b)

Moreover, the matrices for site 1 to any site $\ell = 1, \ldots, N$ define an <u>orthonormal state space</u>:

$$|\Psi_\lambda\rangle_\ell = |\sigma_1\rangle\otimes|\sigma_2\rangle\otimes\ldots\otimes|\sigma_\ell\rangle\,[A_1^{\sigma_1}A_2^{\sigma_2}\ldots A_\ell^{\sigma_\ell}]^1{}_\lambda \qquad (5)$$



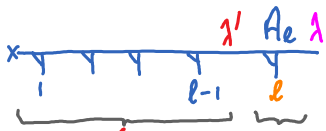
$$_\ell\langle\Psi^{\lambda'}|\Psi_\lambda\rangle_\ell = \mathbb{1}^{\lambda'}{}_\lambda \qquad (6)$$

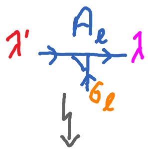
Call this state space $\mathbb{V}_\ell = \mathrm{span}\{|\Psi_\lambda\rangle_\ell\} \subseteq \mathbb{V}_1\otimes\mathbb{V}_2\otimes\ldots\otimes\mathbb{V}_\ell$ (7)

where $\mathbb{V}_\ell = \mathrm{span}\{|\sigma_\ell\rangle\}$ is local state space of site ℓ

These state spaces are built up iteratively from left to right through left-isometric maps:

Each A_ℓ defines an isometric map to a new (possibly smaller) basis:





$$A_\ell : \mathbb{V}_{\ell-1}\otimes\mathbb{V}_\ell \to \mathbb{V}_\ell, \qquad \underbrace{|\Psi_{\lambda'}\rangle_{\ell-1}|\sigma_\ell\rangle}_{\text{old basis}} \mapsto \underbrace{|\Psi_\lambda\rangle_\ell}_{\text{new basis}} = |\Psi_{\lambda'}\rangle_{\ell-1}|\sigma_\ell\rangle [A_\ell]^{\lambda'\sigma_\ell}{}_\lambda \qquad (8)$$

If A_ℓ is a unitary, then $\dim(\mathbb{V}_\ell) = \dim(\mathbb{V}_{\ell-1})\cdot\dim(\mathbb{V}_\ell) \Rightarrow$ no truncation (9)

$$D_\ell = D_{\ell-1}\cdot d$$

If A_ℓ is a (non-unitary) isometry, then $D_\ell < D_{\ell-1}\cdot d \Rightarrow$ truncation was involved! (10)

Hence $\mathbb{V}_\ell = \mathbb{V}_1\otimes\mathbb{V}_2\otimes\ldots\otimes\mathbb{V}_\ell$ only if all A's are not only isometries but unitaries.

$D_\ell = d^\ell$

truncation possible

no truncation!

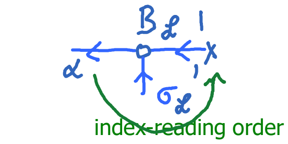
Even if truncation is involved, the resulting MPS are useful, precisely because they are parametrized by a limited number of parameters (namely elements of A tensors). E.g., they can be optimized variationally by minimizing energy $\Rightarrow$DMRG).

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, using left-pointing arrows.

Building blocks:

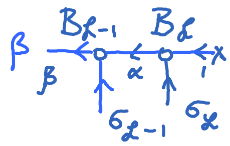
$$|\alpha\rangle = |\sigma_\ell\rangle [B_\ell]_\alpha{}^{\sigma_\ell 1}$$



(11)

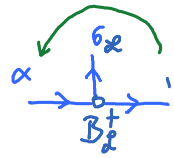
left-to-right index order as in diagram

$$|\beta\rangle = |\sigma_{\ell-1}\rangle|\sigma_\ell\rangle [B_{\ell-1}]_\beta{}^{\sigma_{\ell-1}\alpha} [B_\ell]_\alpha{}^{\sigma_\ell 1}$$



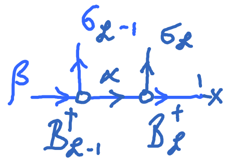
(12)

$$\langle\alpha| = \underbrace{[B^\dagger_\ell]_{1\sigma_\ell}{}^{\alpha}}_{:=\overline{[B_\ell]_\alpha{}^{\sigma_\ell 1}}} \langle\sigma_\ell|$$



(13)

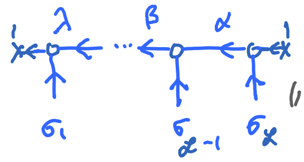
$$\langle\beta| = [B^\dagger_\ell]_{1\sigma_\ell}{}^{\alpha} [B^\dagger_{\ell-1}]_{\alpha\sigma_{\ell-1}}{}^{\beta} \langle\sigma_\ell|\langle\sigma_{\ell-1}|$$



(14)

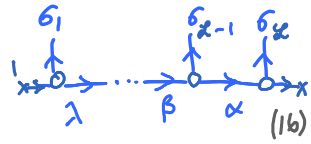
Iterating this, we obtain kets and bras of the form

$$|\psi\rangle = |\sigma_1\rangle|\sigma_2\rangle\ldots|\sigma_\ell\rangle \underbrace{[B_1]_1{}^{\sigma_1\lambda}}\ldots\underbrace{[B_{\ell-1}]_\beta{}^{\sigma_{\ell-1}\alpha}}\underbrace{[B_\ell]_\alpha{}^{\sigma_\ell 1}}$$
$$= |\vec{\sigma}\rangle [B_1^{\sigma_1}\ldots B_{\ell-1}^{\sigma_{\ell-1}} B_\ell^{\sigma_\ell}]_1{}^1$$



(15)

$$\langle\psi| = [B^\dagger_\ell]_{1\sigma_\ell}{}^{\alpha}\underbrace{[B^\dagger_{\ell-1}]_{\alpha\sigma_{\ell-1}}{}^{\beta}}\underbrace{\quad}\ldots\underbrace{[B_1]_{\lambda\sigma_1}{}^{1}}\langle\sigma_\ell|\ldots\langle\sigma_2|\langle\sigma_1|$$
$$= [B_\ell^{\dagger\sigma_\ell} B_{\ell-1}^{\dagger\sigma_{\ell-1}}\ldots B_1^{\dagger\sigma_1}]_1{}^1\langle\vec{\sigma}|$$



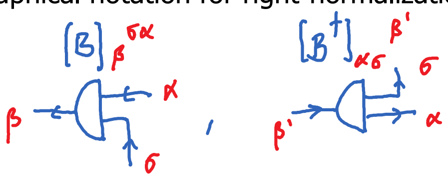
(16)

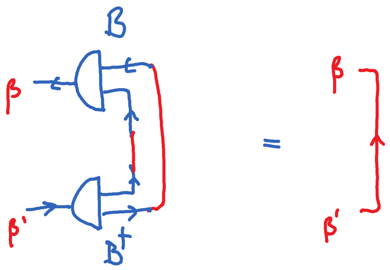
A three-leg tensor $B_\beta{}^{\sigma\alpha}$ is called right-normalized if it is a right isometry, i.e. if it satisfies

$$BB^\dagger = \mathbb{1}. \qquad \text{Explicitly:} \qquad (BB^\dagger)_\beta{}^{\beta'} = B_\beta{}^{\sigma\alpha} B^\dagger_{\alpha\sigma}{}^{\beta'} = \mathbb{1}_\beta{}^{\beta'} \qquad (17)$$

Such a $B^\dagger$ defines an 'isometry' from space labeled by its right indices to space labeled by its left indices.

Graphical notation for right-normalization:





(18a)

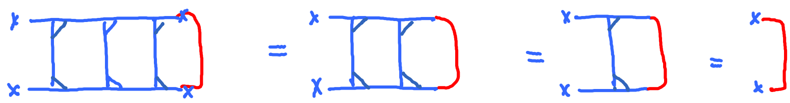
More compact notation: draw 'right-facing diagonals' at vertices

(18b)

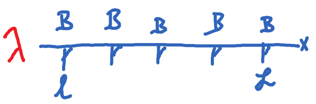
(18b)

Again, right-angled triangles complete information on arrows, so arrows can be suppressed.

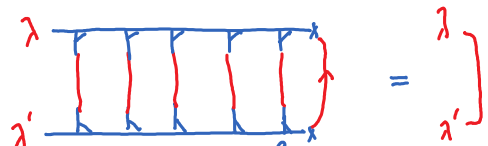
For 'right-normalized MPS', constructed purely from right isometries, closing zipper right-to-left is easy:

$\langle\psi|\psi\rangle =$  $= 1$ (19)

Moreover, the matrices for site $\mathscr{L}$ to any site $\ell = 1, \ldots, \mathscr{L}$ define an orthonormal state space:



$$|\Phi_\lambda\rangle_\ell = |\sigma_\ell\rangle\otimes\ldots\otimes|\sigma_{\mathscr{L}}\rangle \big[B^{\sigma_\ell}_\ell B^{\sigma_{\ell+1}}_{\ell+1}\cdots B^{\sigma_{\mathscr{L}}}_{\mathscr{L}}\big]^{\,1}_{\lambda} \quad (20)$$



close the zipper

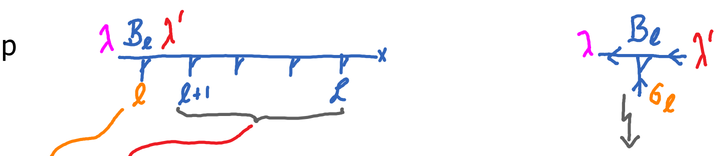
$${}_\ell\langle\Phi^{\lambda'}|\Phi_\lambda\rangle_\ell = \mathbb{1}^{\lambda'}{}_{\lambda} \quad (21)$$

☺

Call this state space $W_\ell = \mathrm{span}\{|\Phi_\lambda\rangle_\ell\} \subseteq V_\ell\otimes V_{\ell+1}\otimes\ldots\otimes V_{\mathscr{L}}$ (22)

These state spaces are built up iteratively from right to left through right-isometric maps:

Each B_ℓ defines an isometric map to a new (possibly smaller) basis:



$$B_\ell : V_\ell\otimes W_{\ell+1}\to W_\ell\,, \qquad \underbrace{|\sigma_\ell\rangle|\Phi_{\lambda'}\rangle_{\ell+1}}_{\text{old basis}} \mapsto \underbrace{|\Phi_\lambda\rangle_\ell}_{\text{new basis}} = |\sigma_\ell\rangle|\Phi_{\lambda'}\rangle_{\ell+1}[B_\ell]^{\sigma_\ell\lambda'}_{\lambda} \quad (23)$$

$W_\ell = V_\ell\otimes V_{\ell+1}\otimes\ldots\otimes V_{\mathscr{L}}$ only if all B's are not only isometries but unitaries. (24)

Summary: 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. ☺

MPS.4 Various canonical MPS forms

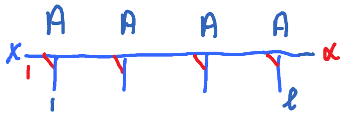
Any matrix product can be expressed in infinitely many different ways without changing the product:

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

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

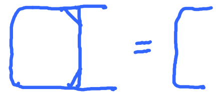
(i) Left-canonical (lc-) MPS:

[all tensors are left-normalized, denoted A]



(2)

$$|\Psi_\alpha\rangle_\ell = |\sigma_1\rangle \dots |\sigma_\ell\rangle \left[A_1^{\sigma_1} \dots A_\ell^{\sigma_\ell}\right]^1{}_\alpha \qquad A^\dagger A = \mathbb{1} \qquad (3)$$



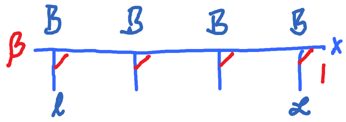
These states form an orthonormal set: $\quad {}_\ell\langle \Psi^{\alpha'} | \Psi_\alpha \rangle_\ell \overset{\text{(MPS-I.2.6)}}{=} \mathbb{1}^{\alpha'}{}_\alpha \qquad (4)$

In general, $\mathbb{V}_\ell \subset \mathcal{H}^\ell$.

true subset

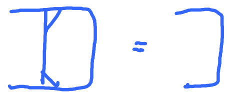
(ii) Right-canonical (rc-) MPS:

[all tensors are right-normalized, denoted B]



(5)

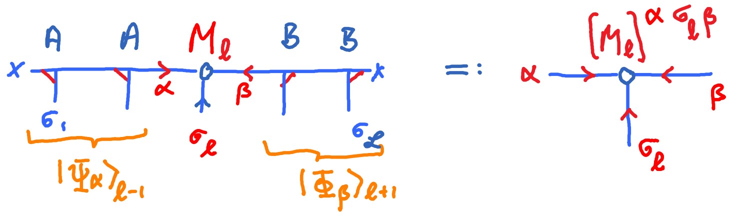
$$|\Phi_\beta\rangle_\ell = |\sigma_\ell\rangle \dots |\sigma_{\mathscr{L}}\rangle \left[B_\ell^{\sigma_\ell} \dots B_{\mathscr{L}}^{\sigma_{\mathscr{L}}}\right]_\beta{}^1 \qquad B B^\dagger = \mathbb{1} \qquad (6)$$



These states form an orthonormal set: $\quad {}_\ell\langle \Phi^{\beta'} | \Phi_\beta \rangle_\ell \overset{\text{(MPS-I.2.18)}}{=} \mathbb{1}^{\beta'}{}_\beta \qquad (7)$

(iii) Site-canonical (sc-) MPS:

[left-normalized to left of site ℓ ,
right-normalized to right of site ℓ]



(8)

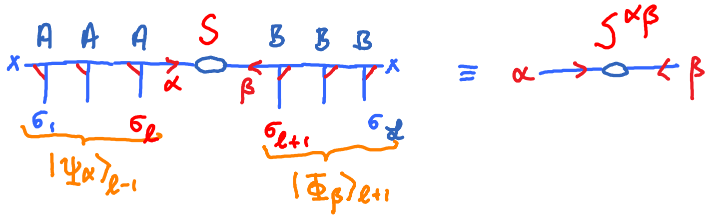
$$|\Psi\rangle = |\vec{\sigma}\rangle_{\mathscr{L}} \left[A_1^{\sigma_1}\dots A_{\ell-1}^{\sigma_{\ell-1}}\right]^1{}_\alpha [M_\ell]^{\alpha\sigma_\ell\beta} \left[B_{\ell+1}^{\sigma_{\ell+1}}\dots B_{\mathscr{L}}^{\sigma_{\mathscr{L}}}\right]_\beta{}^1 = |\Psi_\alpha\rangle_{\ell-1}|\sigma_\ell\rangle|\Phi_\beta\rangle_{\ell+1} [M_\ell]^{\alpha\sigma_\ell\beta} \qquad (9)$$

The states $|\alpha,\sigma,\beta\rangle := |\Psi_\alpha\rangle_{\ell-1}|\sigma_\ell\rangle|\Phi_\beta\rangle_{\ell+1}$ form an orthonormal set: $\langle\alpha',\sigma',\beta'|\alpha,\sigma,\beta\rangle = \mathbb{1}^{\alpha'}{}_\alpha \mathbb{1}^{\sigma'}{}_\sigma \mathbb{1}^{\beta'}{}_\beta$ (10)

$M^{\alpha\sigma_\ell\beta}$ can be viewed as the wavefunction of $|\Psi\rangle$ in this basis.

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

[left-normalized from sites 1 to ℓ ,
right-normalized from sites $\ell+1$ to N]



(11)

$$|\psi\rangle = |\vec{\sigma}\rangle_{\mathcal{L}} \underbrace{[A_1 \dots A_\ell]^{1\sigma_1 \cdots \sigma_\ell}{}_{\alpha}}_{|\Psi_\alpha\rangle_{\ell-1}} S^{\alpha\beta} \underbrace{[B_{\ell+1}^{\sigma_{\ell+1}} \dots B_{\mathcal{L}}^{\sigma_{\mathcal{L}}}]_{\beta}{}^{1}}_{|\Phi_\beta\rangle_{\ell+1}} = \sum_{\alpha\beta} |\Psi_\alpha\rangle_{\ell-1} |\Phi_\beta\rangle_{\ell+1} S^{\alpha\beta} \qquad (12)$$

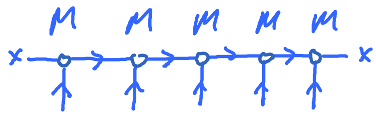
can be chosen diagonal

The states $|\alpha,\beta\rangle := |\Psi_\alpha\rangle_\ell \, |\Phi_\beta\rangle_{\ell+1}$ form an orthonormal set: $\langle\alpha',\beta'|\alpha,\beta\rangle = \mathbb{1}^{\alpha'}{}_{\alpha} \, \mathbb{1}^{\beta'}{}_{\beta}$ (13)

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

Transforming to left-normalized form

Given: $|\psi\rangle = |\vec{\sigma}\rangle_{\mathcal{L}} [M_1 \; \dots \; M_{\mathcal{L}}]^{1\vec{\sigma}}{}_{1}$,

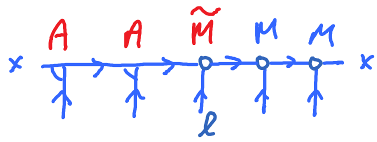


(5)

[or with index: $|\Psi_\alpha\rangle =$ 

]

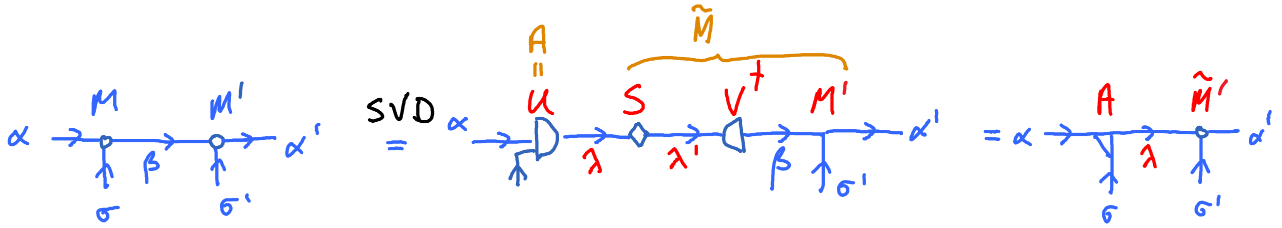
Goal : left-normalize M_1 to $M_{\ell-1}$



(6)

Strategy: take a pair of adjacent tensors, $M M'$, and use SVD to yield left isometry on the left:

$$M M' = U S V^\dagger M' =: A \tilde{M}', \quad \text{with} \quad A := U, \quad \tilde{M}' := S V^\dagger M' \qquad (7)$$



(8)

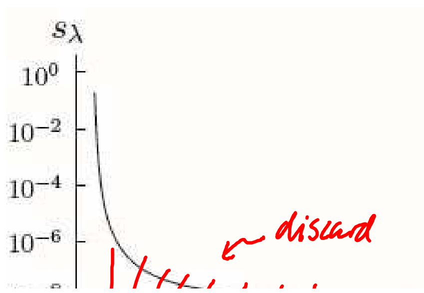
$$M^{\alpha\sigma}{}_{\beta} \; M'^{\beta\sigma'}{}_{\alpha'} = \left(U^{\alpha\sigma}{}_{\lambda}\right)\left(S^{\lambda}{}_{\lambda'} \, V^{\dagger\lambda'}{}_{\beta} \, M'^{\beta\sigma'}{}_{\alpha'}\right) = A^{\alpha\sigma}{}_{\lambda} \, \tilde{M}'^{\lambda\sigma'}{}_{\alpha'} \qquad (9)$$

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

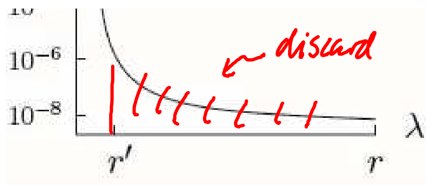
Truncation, if desired, can be performed by discarding some of the smallest singular values, using $U S V^\dagger \approx u s v^\dagger$

$$\sum_{\lambda=1}^{r} \longrightarrow \sum_{\lambda=1}^{r'}$$

(but (10) remains valid!)



$\sum_{\lambda=1} \to \sum_{\lambda=1}$ (but (10) remains valid!)



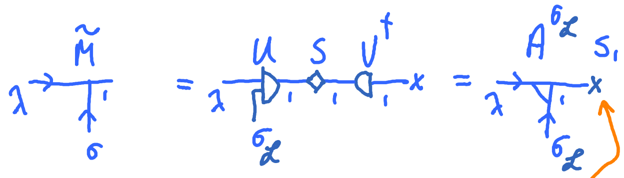
Note: instead of SVD, we could also me QR (cheaper!)

By iterating, starting from $M_1 \; M_2$, we left-normalize M_1 to $M_{\ell-1}$,

To left-normalize the entire MPS, choose $\ell = \mathcal{L}$.

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

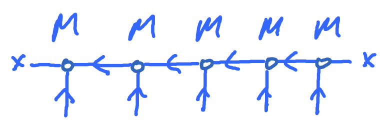
$$\tilde M^{\lambda\sigma_\mathcal{L}}{}_1 = \underbrace{U^{\lambda\sigma_\mathcal{L}}{}_1}_{A^{\lambda\sigma_\mathcal{L}}{}_1} \underbrace{S^1{}_1}_{s_1} \underbrace{V^{\dagger 1}{}_1}_{1} \qquad (11)$$



lc-form: $|\psi\rangle = |\vec\sigma\rangle_\mathcal{L} [A_1^{\sigma_1} \dots A_\mathcal{L}^{\sigma_\mathcal{L}}]^1 \; s_1$

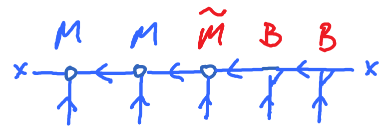
The final singular value, s_1 determines normalization: $\langle\psi|\psi\rangle = |s_1|^2$. (12)

<u>Transforming to right-normalized form</u>



Given: $|\psi\rangle = |\vec\sigma\rangle_\mathcal{L} (M_1^{\sigma_1} \dots M_\mathcal{L}^{\sigma_\mathcal{L}})$

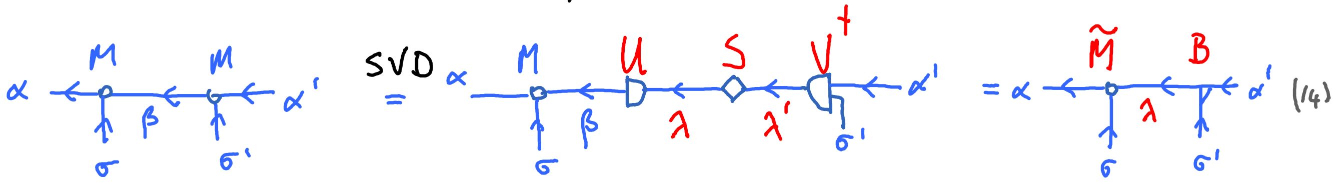
[or with index: $|s_1\rangle =$ ]



Goal : right-normalize $M_\mathcal{L}$ to $M_{\ell+1}$

Strategy: take a pair of adjacent tensors, MM', and use SVD to yield right isometry on the right:

$$MM' = MUSV^\dagger \equiv \tilde M B, \quad \text{with} \quad \tilde M = M'US, \quad B = V^\dagger. \qquad (13)$$



$$M_\alpha{}^{\sigma\beta}\, M'_\beta{}^{\sigma'\alpha'} = \left(M_\alpha{}^{\sigma\beta}\, U_\beta{}^{\lambda}\, S_\lambda{}^{\lambda'}\right)\left(V^\dagger{}_{\lambda'}{}^{\sigma'\alpha'}\right) = \tilde{M}_\alpha{}^{\sigma\lambda'}\, B_{\lambda'}{}^{\sigma'\alpha'} \qquad (15)$$

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

Starting form $M_{\ell-1}\ M_\ell$, move leftward up to $M_\ell\ M_{\ell+1}$.

To right-normalize entire chain, choose / and at last site, $\ell = 1$

$$\tilde{M}_1{}^{\sigma_1\lambda} = \underbrace{U_1{}^1}_{=1}\underbrace{S_1{}^1}_{S_1}\underbrace{V^\dagger{}_1{}^{\sigma_1\lambda}}_{B_1{}^{\sigma_1\lambda}} .$$ S_1 determines normalization. (17)

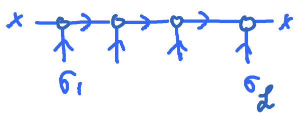
Summary: using SVD, products of two matrices can be converted into forms containing a left isometry on the left or right isometry on the right:

$$M M' = A \tilde{M}' = \tilde{M} B \qquad (18)$$

This can be used iteratively to convert any of the four canonical forms into any other one.

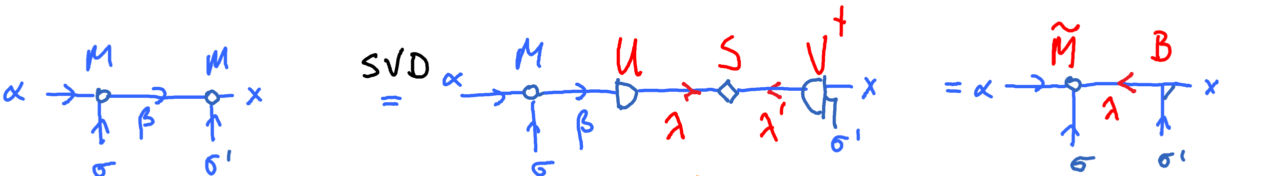
<u>Examples</u> [self-study!]

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



Hint: start at $M_{\ell-1}\ M_\ell$

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

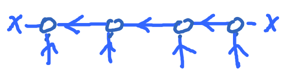


(19a)

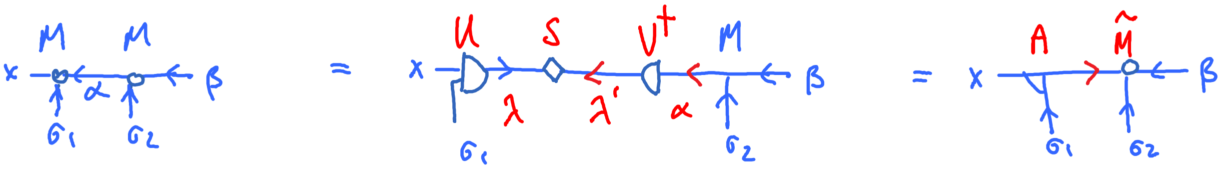
both indices upstairs!

$$M^{\alpha\sigma}{}_\beta\, M^{\beta\sigma'}{}_1 = \left(M^{\alpha\sigma}{}_\beta\, U^\beta{}_\lambda\, S^{\lambda\lambda'}\right)\left(V^\dagger{}_{\lambda'}{}^{\sigma'}\right) = \tilde{M}^{\alpha\sigma\lambda}\, B_\lambda{}^{\sigma'} \qquad (19b)$$

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



Hint: start at $M_1\ M_2$:

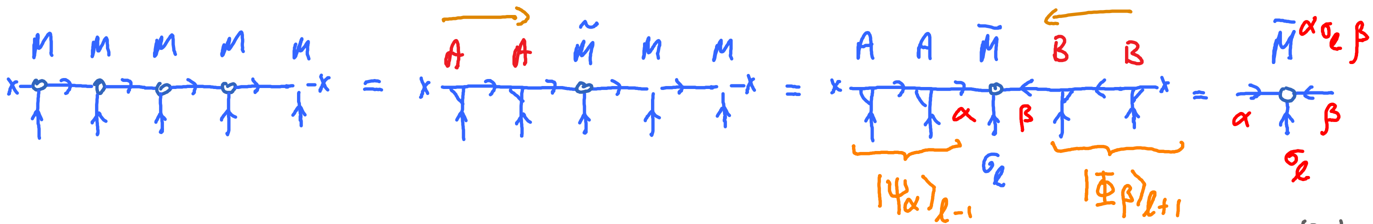


(20)

both indices upstairs!

$$M_1^{\;\sigma_1\alpha}\, M_\alpha^{\;\sigma_2\beta} = \left(U^{1\sigma_1}{}_{\lambda}\right)\left(\overset{\text{both indices upstairs!}}{S^{\lambda\lambda'}}\, V^{\dagger}{}_{\lambda'}{}^{\alpha} M_\alpha^{\;\sigma_2\beta}\right) = A_1^{\;\sigma_1\lambda}\, \tilde{M}_\lambda^{\;\sigma_2\beta} \qquad (21)$$

(c) Transforming to site-canonical form



(22)

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

Then right-normalize sites $\mathcal{L}$ to $\ell+1$, starting from site $\mathcal{L}$.

Result:

$$|\psi\rangle = \underbrace{|\sigma_1\rangle \dots |\sigma_{\ell-1}\rangle \left[A_1^{\sigma_1} \dots A_{\ell-1}^{\sigma_{\ell-1}}\right]^1{}_\alpha}_{|\Psi_\alpha\rangle_{\ell-1}} |\sigma_\ell\rangle \underbrace{|\sigma_{\ell+1}\rangle \dots |\sigma_{\mathcal{L}}\rangle \left[B_{\ell+1}^{\sigma_{\ell+1}} \dots B_{\mathcal{L}}^{\sigma_{\mathcal{L}}}\right]_\beta{}^1}_{|\Phi_\beta\rangle_{\ell+1}} \bar{M}^{\alpha\sigma_\ell\beta} \qquad (23)$$

$$= |\Psi_\alpha\rangle_{\ell-1} |\sigma_\ell\rangle |\Phi_\beta\rangle_{\ell+1}\, \bar{M}^{\alpha\sigma_\ell\beta} \qquad (24)$$

The states $|\alpha, \sigma_\ell, \beta\rangle := |\Psi_\alpha\rangle_{\ell-1} |\sigma_\ell\rangle |\Phi_\beta\rangle_{\ell+1}$ form an orthonormal set:

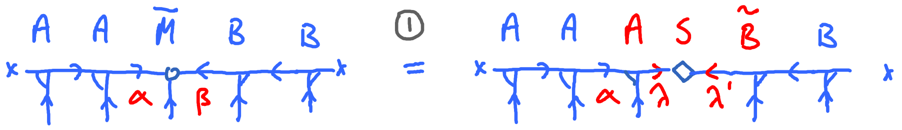
$$\langle \alpha', \sigma_\ell', \beta' | \alpha, \sigma_\ell, \beta\rangle = \delta^{\alpha'}{}_{\alpha}\, \delta^{\sigma_\ell'}{}_{\sigma_\ell}\, \delta^{\beta'}{}_{\beta} \qquad (25)$$

(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 $\lll d^{\mathcal{L}}$ of full Hilbert space.

(d) 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.



$$= \underbrace{|\Psi_\lambda\rangle_\ell}_{\substack{\text{involves}\\ \text{sites } 1 \text{ to } \ell}} \cdot \underbrace{|\Phi_{\lambda'}\rangle_{\ell+1}}_{\substack{\text{involves}\\ \text{sites } \ell+1 \text{ to } \mathcal{L}}} S^{\lambda\lambda'} \qquad (26)$$

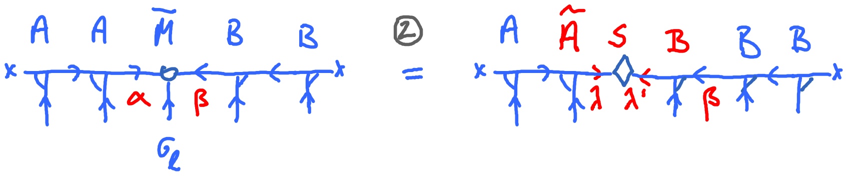
$$\bar{M} = USV^\dagger \qquad A = U, \quad \tilde{B} = V^\dagger B \qquad \text{(Exercise: add indices!)} \qquad (27)$$

The states $|\lambda,\lambda'\rangle := |\Psi_\lambda\rangle_\ell \cdot |\Phi_{\lambda'}\rangle_{\ell+1}$ form an orthonormal set.

$$\langle\bar\lambda,\bar\lambda'|\lambda,\lambda'\rangle = \delta^{\bar\lambda}_{\lambda}\,\delta^{\bar\lambda'}_{\lambda'} \tag{28}$$

This is called the 'local bond basis for bond ℓ' (from site ℓ to $\ell+1$). It has dimension $r\cdot r$

(r = dimension of singular matrix S).



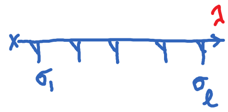
$$= \underbrace{|\Psi_\lambda\rangle_{\ell-1}}_{\text{involves sites } 1 \text{ to } \ell-1}\cdot\underbrace{|\Phi_{\lambda'}\rangle_\ell}_{\text{involves sites } \ell \text{ to } \mathcal{L}}\, S^{\lambda\lambda'} \tag{29}$$

$\tilde M = USV^\dagger$ $\qquad$ $\tilde A = AU$, $\; B = V^\dagger$ $\qquad$ (Exercise: add indices!) (30)

$|\lambda,\lambda'\rangle := |\Psi_\lambda\rangle_{\ell-1} \cdot |\Phi_{\lambda'}\rangle_\ell$ form 'local bond basis' for bond $\ell-1$ (from site $\ell-1$ to ℓ).

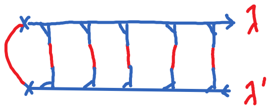
MPS.5 Basis change, projectors

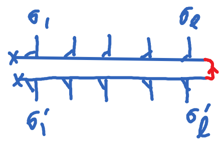
MPS.5

Recall: a set of MPS $|\Psi_\lambda\rangle_\ell = |\sigma_1\rangle\otimes\ldots\otimes|\sigma_\ell\rangle\,[A_1^{\sigma_1}\ldots A_\ell^{\sigma_\ell}]^1{}_\lambda$ =  (1)

specified by given left-normalized tensors

defines an orthonormal basis for a state space $\mathbb{V}_\ell = \mathrm{span}\{|\Psi_\lambda\rangle_\ell\} \subseteq \mathbb{V}_1\otimes\mathbb{V}_2\otimes\ldots\otimes\mathbb{V}_\ell =: \mathbb{V}^{\otimes\ell}$ (2)

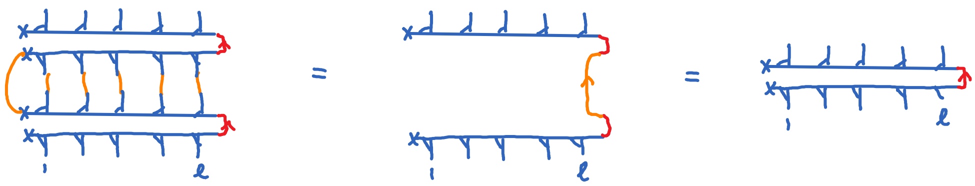
since ${}_\ell\langle\Psi^{\lambda'}|\Psi_\lambda\rangle_\ell$ =  $\overset{\text{close zipper}}{=}$  $= \mathbb{1}^{\lambda'}{}_\lambda$ (3)

Projector onto $\mathbb{V}_\ell$: $\hat P_\ell = |\Psi^\lambda\rangle_\ell\,{}_\ell\langle\Psi_\lambda|$ =  (4)

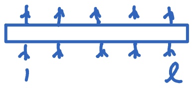
(sum over λ implied)

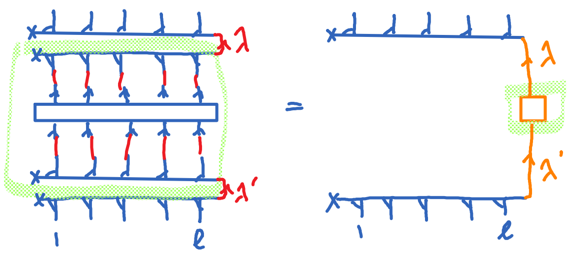
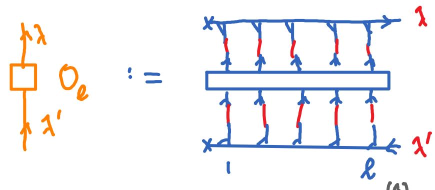
Indeed:

$$\hat P_\ell\,\hat P_\ell = |\Psi^{\lambda'}\rangle_\ell \underbrace{{}_\ell\langle\Psi_{\lambda'}|\cdot|\Psi^{\lambda}\rangle_\ell}_{\mathbb{1}_{\lambda'}{}^{\lambda}} {}_\ell\langle\Psi_\lambda| = \hat P_\ell \quad ✓ \tag{5}$$

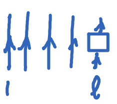
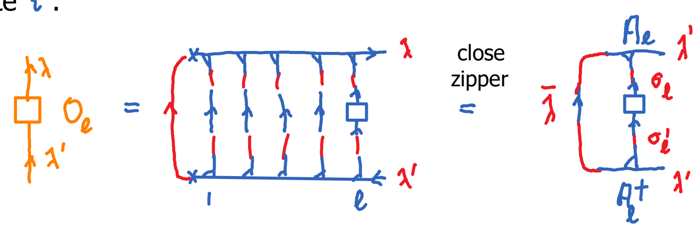
=  (6)

Operators defined on $\mathbb{V}_\ell^{\otimes\ell}$ can be mapped to $\mathbb{V}_\ell$ using these projectors:

$\hat O$ =  $\xmapsto{\hat P_\ell}$ $\hat O_\ell =: \hat P_\ell\,\hat O\,\hat P_\ell =: |\Psi_{\lambda'}\rangle_\ell\,[O_\ell]^{\lambda'}{}_\lambda\,{}_\ell\langle\Psi^\lambda|$ (7)

$\hat O_\ell$ =  , $[O_\ell]^{\lambda'}{}_\lambda$:=  (8)

Simplest case: 1-site operator acting only on site ℓ :

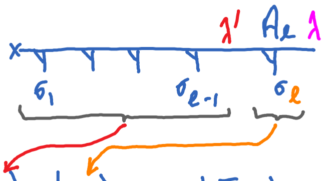
$\hat O_\ell$ =  , $[O_\ell]^{\lambda'}{}_\lambda$ =  (9)

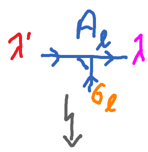
During iterative diagonalization, the space $\mathbb{V}_\ell$ is constructed through a sequence of isometric maps:

(possibly involving truncation)

(possibly involving truncation)

Each  defines an isometric map to a new (possibly smaller) basis:



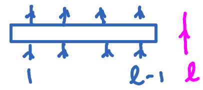


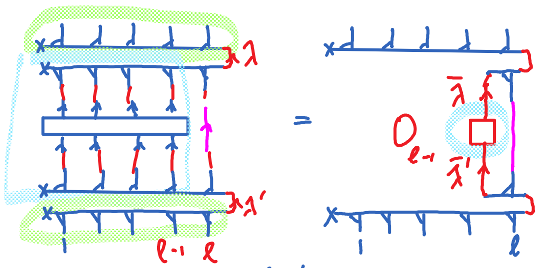
$$A_\ell : \mathbb{V}_{\ell-1} \otimes \mathbb{V}_\ell \to \mathbb{V}_\ell , \qquad |\Psi_{\lambda'}\rangle_{\ell-1} |\sigma_\ell\rangle \mapsto |\Psi_\lambda\rangle_\ell = |\Psi_{\lambda'}\rangle_{\ell-1} |\sigma_\ell\rangle \, [A_\ell]^{\lambda'\sigma_\ell}{}_\lambda \qquad (10)$$

old basis new basis

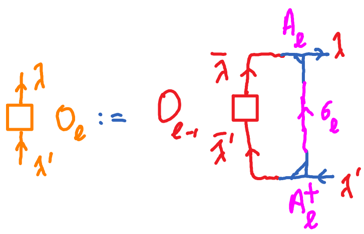
Each such map also induces a transformation of operators defined on its domain of definition.
It is useful to have a graphical depiction for how operators transform under such maps.

Consider an operator defined on $\mathbb{V}^{\otimes(\ell-1)}$, represented on $\mathbb{V}_{\ell-1}$ by $\hat{O}_{\ell-1} = \hat{P}_{\ell-1} \hat{O} \hat{P}_{\ell-1}$ (11)

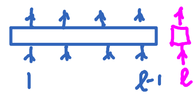
What is its representation on $\mathbb{V}_\ell$? $\hat{O} = \hat{O}_{\ell-1} \otimes \mathbb{1}_\ell =$  (12)

$\hat{O}_\ell =$ 

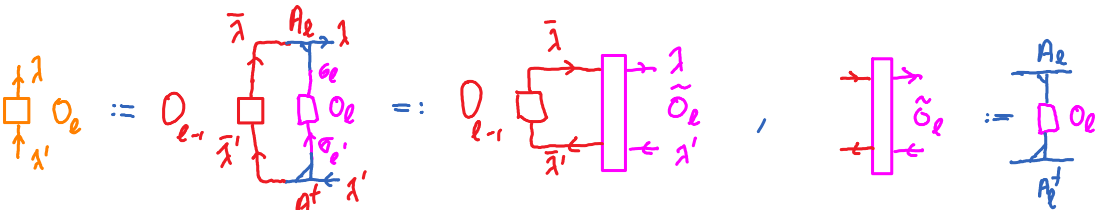
sum on λ, λ' implied

, $[O_\ell]^{\lambda'}{}_\lambda :=$  (13)

Explicitly: $\hat{O}_\ell = |\Psi_\lambda\rangle_\ell \, [O_\ell]^\lambda{}_{\lambda'} \, {}_\ell\langle \Psi^{\lambda'}|$, $\quad [O_\ell]^{\lambda'}{}_\lambda = A^{\dagger\lambda'}{}_{\sigma_\ell\bar\lambda'} \, [O_{\ell-1}]^{\bar\lambda'}{}_{\bar\lambda} \, A^{\bar\lambda\sigma_\ell}{}_\lambda$ (14)

Similarly, for operator with non-trivial action also on site : $\hat{O}_\ell = \hat{O}_{\ell-1} \otimes \hat{O}_\ell =$  (15)

Just replace  by  in (9):

$[O_\ell]^{\lambda'}{}_\lambda :=$  (16)

$$= A^{\dagger\lambda'}{}_{\sigma_\ell'\bar\lambda'} \, [O_{\ell-1}]^{\bar\lambda'}{}_{\bar\lambda} \, [O_\ell]^{\sigma_\ell'}{}_{\sigma_\ell} \, A^{\bar\lambda\sigma_\ell}{}_\lambda = [O_{\ell-1}]^{\bar\lambda'}{}_{\bar\lambda} \, [\tilde{O}_\ell]_{\bar\lambda'}{}^{\bar\lambda}{}_{\lambda} \qquad (17)$$

Thus, the isometry A_ℓ maps the local operator into an effective basis associated with $\mathbb{V}_{\ell-1}$ and $\mathbb{V}_\ell$