- Bringing an MPS into canonical forms:

– "left canonization" of generic MPS:

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1}_{1a_1} A^{\sigma_2}_{a_1a_2} \cdots A^{\sigma_L}_{a_{L-1}1} \, |\sigma_1, \dots, \sigma_L\rangle =$$

$$A^{\sigma_1}_{1\,a_1} \overset{\text{SVD}}{=} U_{\sigma_1,s_1} S_{s_1s_1} V^{\dagger}_{s_1a_1}$$

$$U_{\sigma_1,s_1} =: L^{\sigma_1}_{1a_1}$$

$$= \sum_{\{\sigma\}} L^{\sigma_1}_{1s_1} \underbrace{\left(\sum_{a_1} S_{s_1s_1} V^{\dagger}_{s_1a_1} A^{\sigma_2}_{a_1,a_2} \right)}_{=: \tilde{A}^{\sigma_2}_{s_1a_2}} A^{\sigma_3}_{a_2a_3} \cdots A^{\sigma_L}_{a_{L-1}1} \, |\sigma_1, \dots, \sigma_L\rangle$$

$$\tilde{A}^{\sigma_2}_{s_1\,a_2} \xrightarrow{\text{SVD}} = \sum_{\{\sigma\}} L^{\sigma_1}_{1s_1} L^{\sigma_2}_{s_1s_2} \tilde{A}^{\sigma_3}_{s_2a_3} \cdots \, |\sigma_1, \dots, \sigma_L\rangle = \dots$$

$$\ldots = \sum_{\{\sigma\}} L^{\sigma_1}_{1 s_1} L^{\sigma_2}_{s_1 s_2} \cdots L^{\sigma_L}_{s_{L-1} 1} \underbrace{S_{11} V^\dagger_{11}}_{= \text{ scalar } \sim \text{ Norm of } |\psi\rangle} |\sigma_1, \ldots, \sigma_L\rangle$$

↳ Crucial feature of left-canonical MPS (by def. of SVD):

$$\boxed{\sum_{\sigma_j} L^{\sigma_j \dagger} L^{\sigma_j} = \mathbb{1} \quad \forall j}$$

(equivalent to $U^\dagger U = \mathbb{1}$ in SVD)

- "right canonization" of generic MPS: Analogous to left-canonical case, but using $A^\sigma = U S V^\dagger$, where $V^\dagger$ is used to define R^{σ_j} such that

$$|\psi\rangle = \sum_{\{\sigma\}} \underbrace{U_{11} S_{11}}_{\text{scalar} \sim \text{norm } |\psi\rangle} R^{\sigma_1}_{1 s_1} R^{\sigma_2}_{s_1 s_2} \cdots R^{\sigma_L}_{s_{L-1},1} |\sigma_1, \ldots, \sigma_L\rangle$$

with $$\boxed{\sum_{\sigma_j} R^{\sigma_j} R^{\sigma_j \dagger} = \mathbb{1} \quad \forall_j}$$

- Mixed canonical MPS: Left-canonical up to site l, right-canonical from $l+1$ to L:

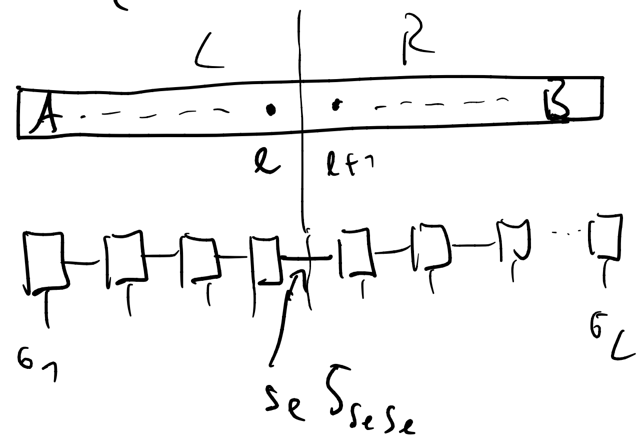
$$|\psi\rangle = \sum_{\{\sigma\}} L^{\sigma_1}_{1 s_1} L^{\sigma_2}_{s_1 s_2} \cdots L^{\sigma_l}_{s_{l-1} s_l} \; S_{s_l s_l} \, R^{\sigma_{l+1}}_{s_l s_{l+1}} \cdots R^{\sigma_{L-1}}_{s_{L-2} s_{L-1}} R^{\sigma_L}_{s_{L-1} 1}$$

↳ With $$|s_l^A\rangle = \sum_{\sigma_1, \ldots \sigma_l} \left(L^{\sigma_1} \cdots L^{\sigma_l}\right)_{1 s_l} |\sigma_1, \ldots, \sigma_l\rangle$$ and

$$|s_l^B\rangle = \sum_{\sigma_{l+1}, \ldots, \sigma_L} \left(R^{\sigma_{l+1}} \cdots R^{\sigma_L}\right)_{s_l 1} |\sigma_{l+1}, \ldots, \sigma_L\rangle,$$

we get $$|\psi\rangle = \sum_{s_\ell} S_{s_\ell s_\ell} |s_\ell^A\rangle \otimes |s_\ell^B\rangle .$$

Graphically:

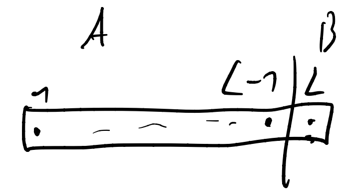


$\rightsquigarrow$ mixed canonical form makes Schmidt decomposition manifest, since $\sum_{\sigma_j} L^{\sigma_j \dagger} L^{\sigma_j} = \mathbb{1}$, $j = 1, \dots \ell$ and $\sum_{\sigma_j} R^{\sigma_j} R^{\sigma_j \dagger} = \mathbb{1}$, $j = \ell+1, \dots, L$ ensure orthonormality of the $\{|s_\ell^A\rangle\}$ and $\{|s_\ell^B\rangle\}$ basis sets.

- Compress MPS by SVD (from bond dim. X to $x < X$)

- Starting point: Left-canonical MPS $|\psi^{(L)}\rangle = \sum_{\{\sigma\}} L^{\sigma_1}\cdots L^{\sigma_L}|\sigma_1\cdots\sigma_L\rangle$

- Basic procedure: Right canonize $|\psi^{(L)}\rangle$ site by site, retaining only the x largest singular values at every SVD step:



$$|\psi^{(L-1)}\rangle = \sum_{\{\sigma\}} L^{\sigma_1}\cdots\cdots L^{\sigma_{L-1}}\, U S R^{\sigma_L}|\sigma_1,\dots,\sigma_L\rangle$$

↳ Read off Schmidt-decomp.: $|s^B_{L-1}\rangle = \sum_{\sigma_L} R^{\sigma_L}_{s_{L-1}1}|\sigma_L\rangle$,

$$|s^A_{L-1}\rangle = \sum_{\sigma_1,\dots,\sigma_{L-1}} \left(L^{\sigma_1}\cdots L^{\sigma_{L-1}}U\right)_{1 s_{L-1}} |\sigma_1,\dots,\sigma_{L-1}\rangle, \quad \text{i.e.}$$

$$|\psi^{(L-1)}\rangle = \sum_{s_{L-1}} S_{s_{L-1}s_{L-1}}\, |s^A_{L-1}\rangle\otimes|s^B_{L-1}\rangle \quad (\text{keep only } s_{L-1}=0,\dots,x)$$

continue from right to left,
at every step, truncate matrices to only keep the
χ largest singular values

until $|\tilde{\psi}\rangle = \sum_{\{\sigma\}} \tilde{R}^{\sigma_1} \ldots \tilde{R}^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle$ is reached.

$\rightsquigarrow$ $|\tilde{\psi}\rangle$ is the compressed MPS of bond dim. χ.

- Problem with SVD compression: Truncation procedure has clear direction that may lead to artefacts for "lossy compressions" (significant singular values being cut).

$\rightsquigarrow$ Cure: More elaborate iterative optimization algorithms for compression (see U. Schollwöck 2011 Review for details)

- Matrix product operators (MPOs)

- Basic idea: By analogy to MPS form

$$\langle \sigma_1, \ldots, \sigma_N | \psi \rangle = A^{\sigma_1} \cdots A^{\sigma_N},$$

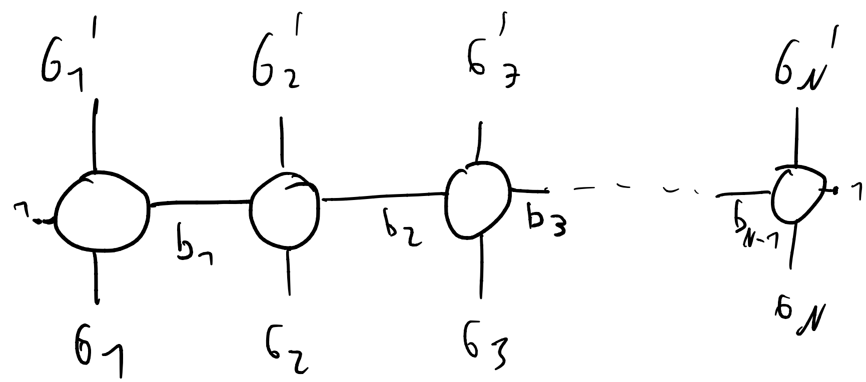
represent

$$\langle \sigma_1, \ldots \sigma_N | O | \sigma_1', \ldots, \sigma_N' \rangle = W^{\sigma_1 \sigma_1'} \cdots W^{\sigma_N \sigma_N'}$$

with matrices $W^{\sigma_j \sigma_j'}_{b_{j-1} b_j}$, resulting in the form

$$O = \sum_{\{\sigma, \sigma'\}} W^{\sigma_1 \sigma_1'}_{1 b_1} W^{\sigma_2 \sigma_2'}_{b_1 b_2} \cdots W^{\sigma_N \sigma_N'}_{b_{N-1} 1} |\sigma_1, \ldots, \sigma_N\rangle \langle \sigma_1', \ldots, \sigma_N'|$$

or graphically

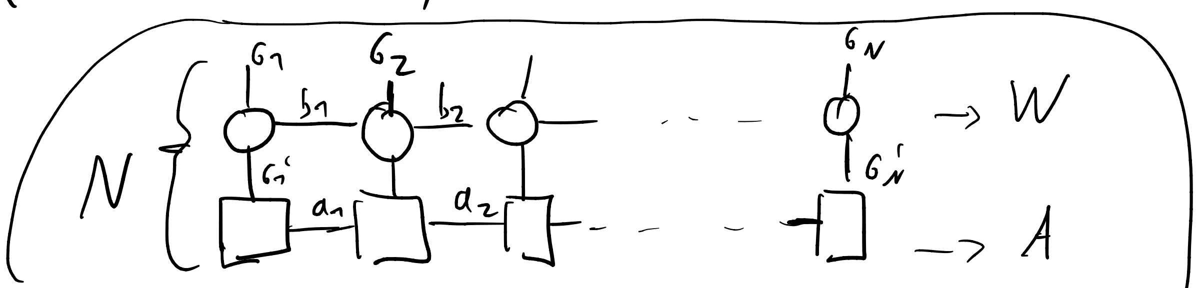


↳ At the expense of a possibly exponentially big bond dimension (size of W matrices for fix physical indices), any operator can be brought into MPO form by successive SVD.

↳ Applying an MPO to an MPS:

$$O|\psi\rangle = \sum_{\{\sigma,\sigma'\}} \left(W^{\sigma\sigma_1'} \cdots W^{\sigma_N\sigma_N'}\right)\left(A^{\sigma_1'} \cdots A^{\sigma_N'}\right)|\sigma_1,\dots,\sigma_N\rangle$$

$$= \sum_{\substack{a_1,\dots,a_{N-1}\\ b_1,\dots,b_{N-1}}} \sum_{\{\sigma,\sigma'\}} \left(W^{\sigma_1\sigma_1'}_{1 b_1} A^{\sigma_1'}_{1 a_1}\right)\left(W^{\sigma_2\sigma_2'}_{b_1 b_2} A^{\sigma_2'}_{a_1 a_2}\right)\cdots\left(W^{\sigma_N\sigma_N'}_{b_{N-1}1} A^{\sigma_N'}_{a_{N-1}1}\right)|\sigma_1\dots\sigma_N\rangle$$

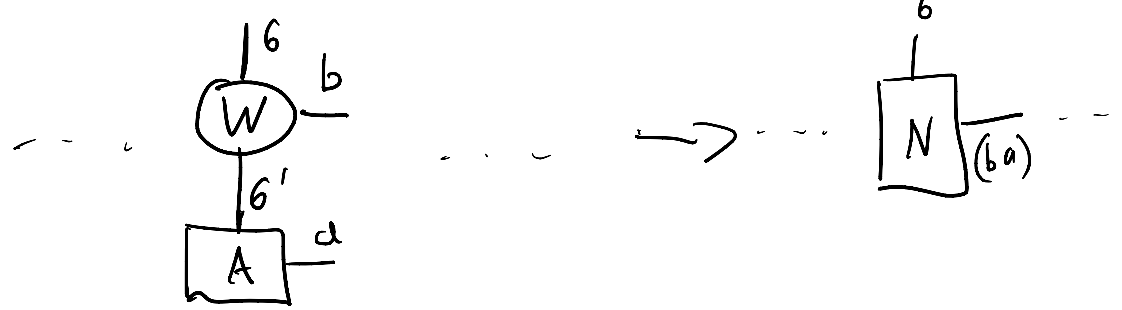


$$= \sum_{b_1 a_1, \dots, b_{N-1} a_{N-1}} \sum_{\{\sigma\}} N^{\sigma_1}_{1(b_1 a_1)} N^{\sigma_2}_{(b_1 a_1)(b_2 a_2)} \cdots N^{\sigma_N}_{(b_{N-1} a_{N-1})1} |\sigma_1, \dots, \sigma_N\rangle,$$

i.e. $O|\psi\rangle$ is MPS with $N^{\sigma_i}_{(b_{i-1} a_{i-1})(b_i a_i)} = \sum_{\sigma_i'} W^{\sigma_i \sigma_i'}_{b_{i-1} b_i} A^{\sigma_i'}_{a_i a_i}$.

$\rightsquigarrow$ The bond dimension of $O|\psi\rangle$ is the <u>product</u> of the bond-dim. of MPS "$|\psi\rangle$" and MPO "O", and the N matrices are tensor products of A and W matrices: $N^{\sigma_i} = \sum_{\sigma_i'} W^{\sigma_i \sigma_i'} \otimes A^{\sigma_i'}$.

i.e.:



In generic algorithms such as tMPS, MPOs with small individual bond dim. are iteratively applied to an MPS, and the resulting MPS is compressed after every step.