Last lecture:

Variational optimization over MPS:

Find best MPS approx. to G.S. of $H = \sum h_i$.

Use: $|\psi\rangle =$ 

$\rightarrow$ $|\psi\rangle$ is linear in each $A^{[s]}$

$\Rightarrow$ minimization of $E(A^{[s]}) = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$ eigenvalue probl.

Important trick: Isometric gauge:

Today: more on numerics w/ MPS.

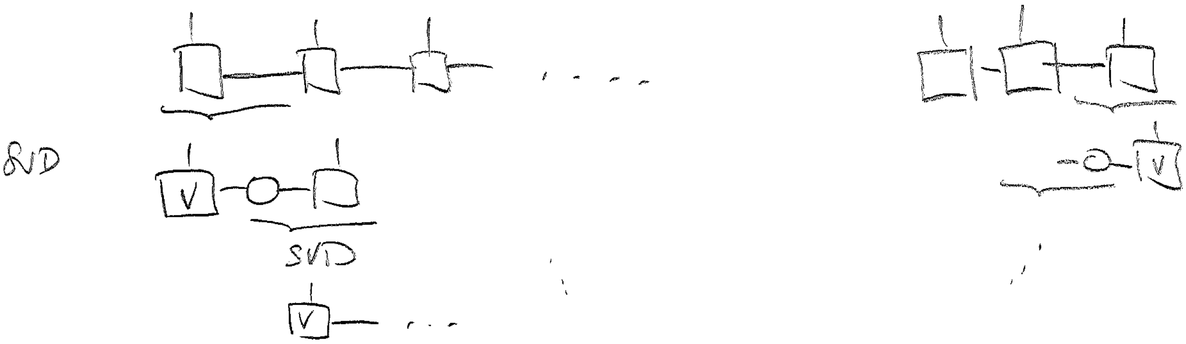
① Truncating the bond dimension

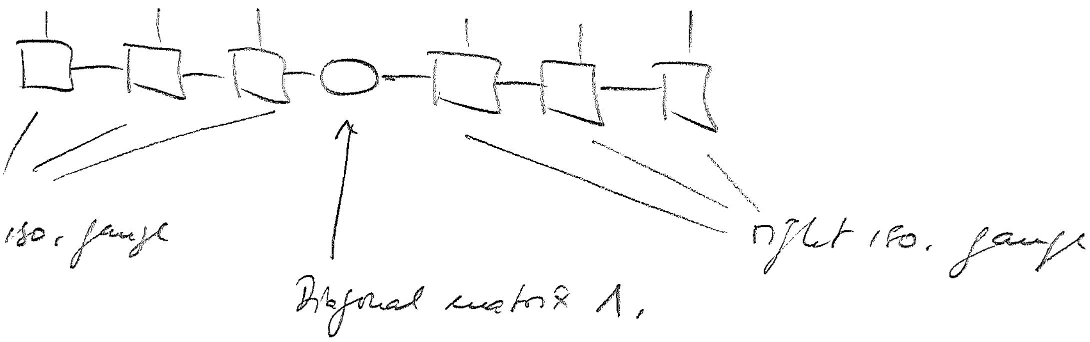
Given MPS $|\psi\rangle$ w/ some D, can we approximate it by an MPS $|\phi\rangle$ with $D' < D$?

Method I: Do it as in DMRG – optimize $B^{[s]}$ (in $|\phi\rangle$) sequentially, s.th. $\dfrac{|\langle\psi|\phi\rangle|^2}{\langle\phi|\phi\rangle}$ becomes maximal $\Rightarrow$ quadr. problem!

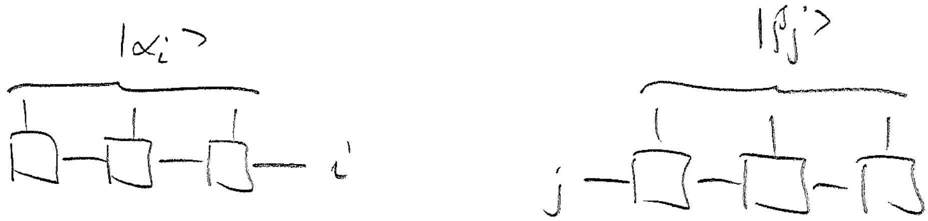
Method II: Truncation

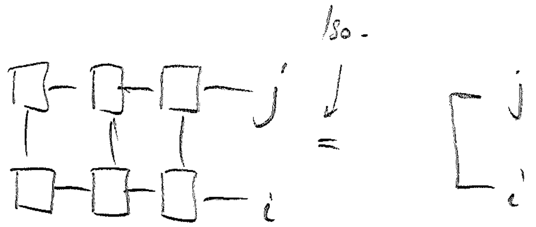
Choose cut s & choose isometric gauge:



$\Rightarrow |\psi\rangle =$ 

Regard left/right as basis:



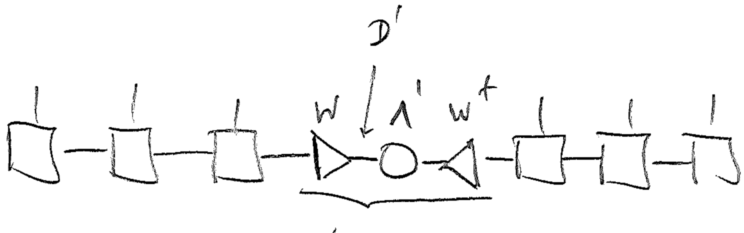
$\langle \alpha_j | \alpha_i \rangle =$  $= \delta_{ij}$

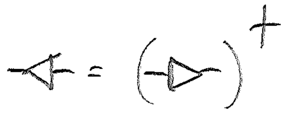
$\Rightarrow |\alpha_i\rangle, |\beta_j\rangle$ orthonormal bases!

$\Rightarrow$ Schmidt decomposition $|\psi\rangle = \sum_{i=1}^{D} \Lambda_{ii} |\alpha_i\rangle |\beta_i\rangle$

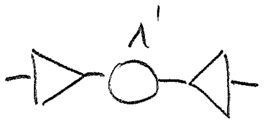
Truncation: Assume wlog $\Lambda_{11} \geq \Lambda_{22} \geq \dots$

$\Rightarrow$ cut there at $D' < D$.



: isometry $\begin{pmatrix} 1 & & & \\ & \ddots & & 0 \\ & & 1 & \end{pmatrix}$. 

$$\Lambda' = \begin{pmatrix} \Lambda_{11} & & \\ & \ddots & \\ & & \Lambda_{D'D'} \end{pmatrix}.$$

$\Rightarrow$  $\approx \Lambda$, and new bond dim. is D'.

What is the error?

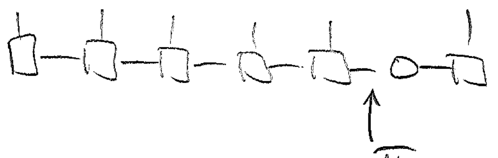
$$\left\| \sum_{i=1}^{D} \Lambda_{ii} |\alpha_i\rangle|\beta_i\rangle - \sum_{i=1}^{D'} \Lambda_{ii} |\alpha_i\rangle|\beta_i\rangle \right\|$$

$$= \left(\sum_{D'+1}^{D} (\Lambda_{ii})^2 \right)^{1/2} =: \varepsilon_s \quad (\text{"tail weight"})$$

Perform this at <u>all</u> cuts.

$\Rightarrow$ Maximal error is $\varepsilon = \sum' \varepsilon_s$.

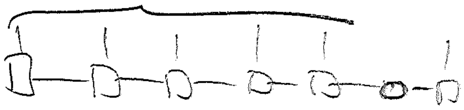
<u>Proof:</u> Consider left iso gauge. Cut = Projection on Bond:



Π_s : ts

Iso gauge: $\Pi_s \hat{=} P_s$:

P_s,



Determine all cuts $\Pi_s \hat{=} P_s$ this way:

$$|\psi_{trunc}\rangle = P_1 \cdot P_2 \cdot \ldots \cdot P_{N-1} |\psi\rangle$$

(since we can sequentially move $P_{N-1}, P_{N-2}, \ldots, P_1$ to $\Pi_{N-1}, \Pi_{N-2}, \ldots$)

<u>And:</u> $$|\psi_{N-1}\rangle = P_{N-1}|\psi\rangle = |\psi\rangle + \underbrace{|\delta\psi_{N-1}\rangle}_{\|\cdot\| = \varepsilon_{N-1}}$$

$$P_{N-2}P_{N-1} = P_{N-2}|\psi_{N-1}\rangle = \underbrace{P_{N-2}|\psi\rangle}_{= |\psi\rangle + \underbrace{|\delta\psi_{N-2}\rangle}_{\|\cdot\| \le \varepsilon_{N-2}}} + \underbrace{P_{N-1}|\delta\psi_{N-1}\rangle}_{\|\cdot\| \le \||\delta\psi_{N-1}\rangle\| = \varepsilon_{N-1}}$$

$$\Rightarrow \| P_1 \ldots P_{N-1}|\psi\rangle - |\psi\rangle \| \le \sum \varepsilon_s . \quad \boxed{}$$

<u>Note:</u> "tail weight" ε_S is related to <u>entanglement entropy</u>:

$$\varepsilon_S^2 = \sum_{D'+1}^{D} \underbrace{\Lambda_{i i}^2}$$

distr. for entropy!

Area law (for S_α, $\alpha<1$) $\Rightarrow$ Λ_{ii}^2 decay quickly $\Rightarrow$

$\varepsilon_S^2 \to 0$ fast as $D' \nearrow \infty$ $\Rightarrow$ efficient approximation.

<u>Note:</u> (i) Faster than seq. optimization, but latter might be better.

(ii) Truncation can also be generalized to transl. invariant infinite systems.

<u>Applications:</u> real/imaginary time evolution:

$H = \sum h_i$. $|\psi_0\rangle$ ground state:

$$|\psi_0\rangle \approx \underbrace{e^{-\beta H}}_{} \underbrace{|+ \dots +\rangle}_{\text{or some other product state...}}$$

required β dep. on properties (gap etc.) of H.

How can we apply $e^{-\beta H}$ efficiently (in a tensor network picture)?

Trotter (Lie-Suzuki-Trotter) decomposition:

Wlog: $H = \sum h_{i,i+1}$

$$\Rightarrow \quad H = \underbrace{\left(\sum_{i=0,2,4,\dots} h_{i,i+1} \right)}_{=: h_{even}} + \underbrace{\left(\sum_{i=1,3,5,\dots} h_{i,i+1} \right)}_{=: h_{odd}}$$

→ terms <u>within</u> h_{even} / h_{odd} mutually commuting!

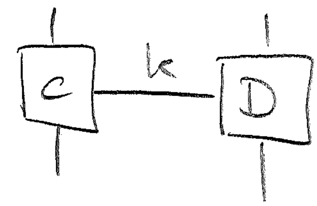
$$\Rightarrow \quad e^{-\beta H} = \left(e^{-\beta H/M} \right)^M \approx \Big(\underbrace{e^{-\beta h_{even}/M}}_{= \prod_{even} e^{-\beta h_{i,i+1}/M}} \; \underbrace{e^{-\beta h_{odd}/M}}_{= \prod_{odd} e^{-\beta h_{i,i+1}/M}} \Big)^M$$

→ product of local operators!

→ error like $O\left(\frac{1}{M}\right)$ – or better for "higher order" Trotter.

Translate to tensor networks:

$$\underbrace{e^{-\beta h_{i,i+1}/M}}_{\text{two-site operator}} = \sum_k C_k \otimes D_k$$

$=$ 

etc.

$e^{-\beta h_{odd}/M}$

$e^{-\beta h_{even}/M}$

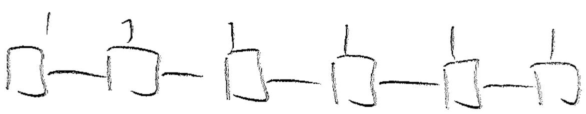
$|\psi_{init}\rangle$

$\Downarrow$ block tensors in column

increased dimension

$\Downarrow$ truncate

$|\psi'\rangle$



$\Rightarrow$ iterate until convergence is reached!

<u>Note:</u> This construction also can give an intuition why MPS approx. G.S. well — it gives a construction for G.S. with large D, but in every $e^{-\beta h_{i,i+1}/M}$, the bond is used "very little" (as we are very close to $\mathbb{1}$) — the bond can be compressed well. ($\rightarrow$ can be turned into a proof)

Similar idea for real time evolution:

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

→ can use again Trotter, ~~truncation~~ etc.

Bad: ① less stable: imag. time evol. goes to G.S. ⇒ "self-correcting"

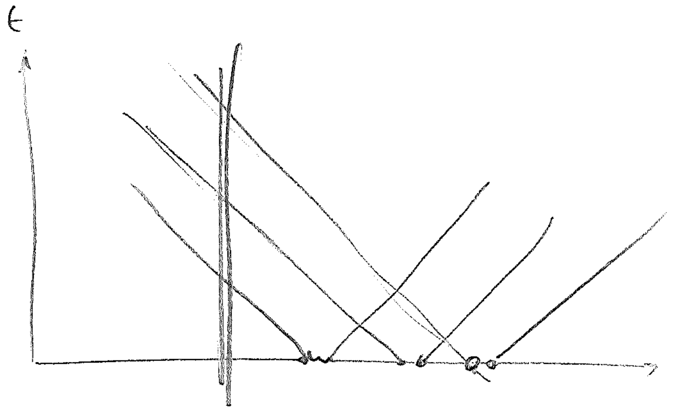
real time evol: unitarity ⇒ errors stay forever.

(Test: evolve + un-evolve: $e^{iHt}\left[e^{-iHt}|\psi(0)\rangle\right] \stackrel{?}{=} |\psi(0)\rangle$?)

Major bottleneck: In time evolution, entropy typ. grows linearly with time: $S(t) \sim t$; i.e., $D \sim \exp(t)$.

Intuition: Initial state has constant density of excitations.

Excit. are ulog entangled + move in opposite direction.



excitations through cut $\sim t$!