Gauge transformation for MPS

Any MPS has a gauge degree of freedom:

$$A^{[i]} \longleftrightarrow X_i A^{[i]} X_{i+1}^{-1}:$$

$$\mathrm{tr}\left[A^{[1]i_1} \cdot A^{[2]i_2} \cdot \ldots \cdot\right] =$$

$$= \mathrm{tr}\left[\underbrace{A^{[1]i_1} X_2^{-1}}_{B^{[1]i_1}} \underbrace{X_2 A^{[2]i_2}}_{B^{[2]i_2}} \ldots \cdot\right] =$$

$$= \text{etc.},$$

$\longleftrightarrow$ many different ways to describe the same state!

* This gauge degree of freedom also exists for OBC!

"Isometric gauge": For an OBC MPS,

the following choice of gauge is part. interesting:

$$\boxed{c_{i_1,\ldots,i_N} = \underbrace{A^{[1]i_1}}_{1\times D} \cdot \underbrace{A^{[2]i_2} \cdot \ldots \cdot A^{[N-1]i_{N-1}}}_{D\times D} \underbrace{A^{[N]i_N}}_{D\times 1}}$$

1. Start from site 1:

* $A^{[1]i_1}$ is $1\times D$ vector: $A_\alpha^{[1]i_1}$.

* Do SVD w.r.t. to indices i_1 and α:

$$A_\alpha^{[1]i_1} = \sum V_\lambda^{[1]i_1} \underbrace{D_{\lambda\lambda}^{(1)} W_{\lambda\alpha}^{(1)}}_{= X_{\lambda\alpha}^{(1)}} \qquad \left(\text{or: } A^{[1]i_1} = V^{[1]i_1} \cdot X^{[1]}\right)$$

Isometry: $\boxed{\sum V_\lambda^{[i]i_1} \bar{V}_{\lambda'}^{[i]i_1} = \delta_{\lambda\lambda'}}$

$$* \quad c_{i_1 \dots i_N} = V^{[1] i_1} \underbrace{\cancel{X}^{(1)} A^{[2] i_2}}_{=: B^{[2] i_2}} \dots A^{[N] i_N}$$

$$= V^{[1] i_1}_{\lambda} B^{[2] i_2} A^{[3] i_3} \dots A^{[N] i_N}$$

2. Go to site 2:

~~SVD: $B^{[2] i_2}$~~

SVD of $B^{[2] i_2}_{\alpha\beta}$ w.r.t. (α, i_2) and β:

one index!

$$B^{[2] i_2}_{\alpha\beta} = \sum V^{[2] i_2}_{\alpha\lambda} \underbrace{D^{(1)}_{\lambda\lambda} W^{[1]}_{\lambda\beta}}_{\equiv X^{[2]}_{\lambda\beta}}$$

$$\left(\text{or: } B^{[2] i_2} = V^{[2] i_2} X^{[2]} \right)$$

with $\boxed{\sum V^{[2] i_2}_{\alpha\lambda} V^{[2] i_2 *}_{\alpha\lambda'} = \delta_{\lambda\lambda'}}$ (Isometry)

$$\Rightarrow c_{i_1, \dots, i_N} = V^{[1] i_1} V^{[2] i_2} \underbrace{X^{[2]} A^{[3] i_3}}_{B^{[3] i_3}} A^{[4] i_4} \dots$$

$$= V^{[1] i_1} V^{[2] i_2} B^{[3] i_3} A^{[4] i_4} \dots$$

3, ..., N-1: Iterate this for site 3, ..., N.

Final outcome:

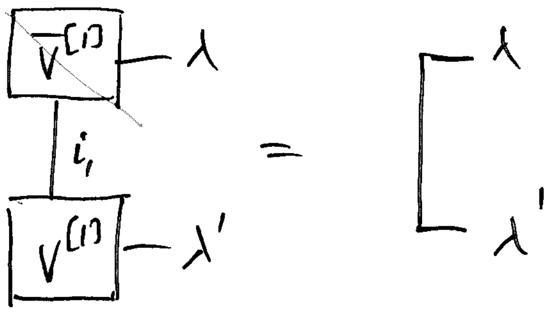
$$c_{i_1,\dots,i_N} = V^{[1]i_1} \cdot V^{[2]i_2} \cdot \dots \cdot V^{[N-1]i_{N-1}} \, V^{[N]i_N}$$

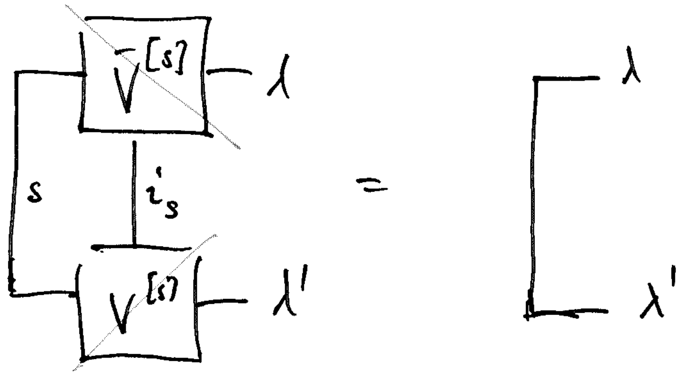
with $\sum V^{[1]i_1}_{\lambda} V^{[1]i_1}_{\lambda'} = \delta_{\lambda\lambda'}$

and $\sum V^{[s]i_s}_{\alpha\lambda} V^{[s]i_s}_{\alpha\lambda'} = \delta_{\lambda\lambda'}$ for $s = 2,\dots,N-1$

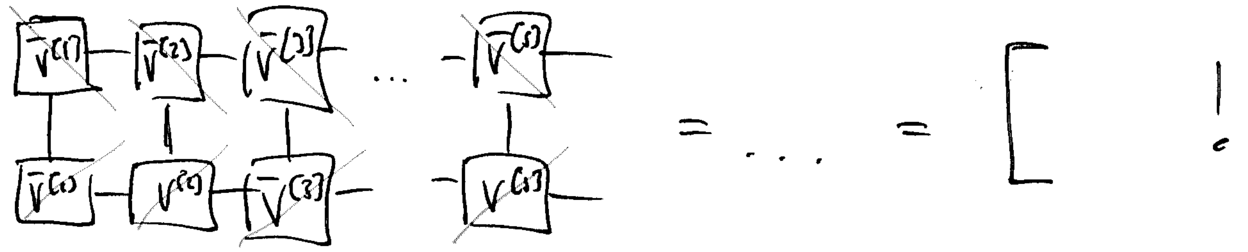
"Isometric gauge"

Graphically:

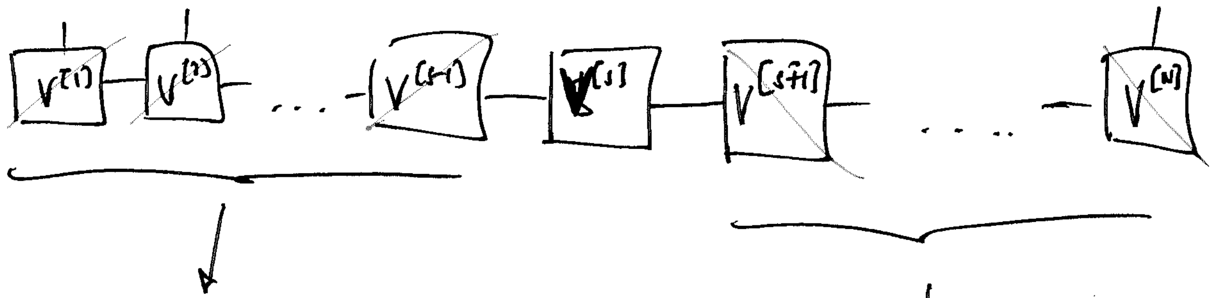




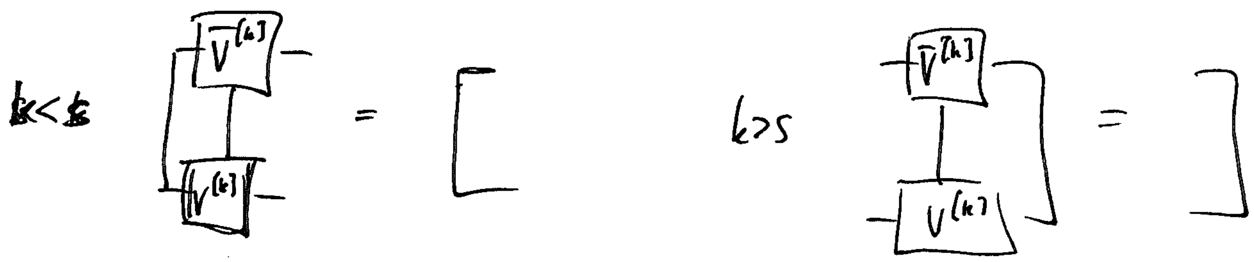
This implies:



It is also possible to start this procedure from left and right, to obtain a form



with



Variational optimization over MPS

(DMRG: Density Matrix Renormalization Group)

How can we find the MPS with the lowest energy for a given local Hamiltonian $H = \sum_i h_{i,i+1}$ (e.g. Ising, Heisenberg)

Basic idea:

1. Start from some initial configuration
$$|\psi\rangle = |\psi[A^{[1]}, A^{[2]}, \dots A^{[N]}]\rangle$$

2. Pick one site s and optimize energy as function:
$$|\psi[X]\rangle = |\psi[A^{[1]}, \dots, A^{[s-1]}, X, A^{[s+1]}, \dots, A^{[N]}]\rangle$$

$$E[X] = \frac{\langle\psi[X]|H|\psi[X]\rangle}{\langle\psi[X]|\psi[X]\rangle}$$

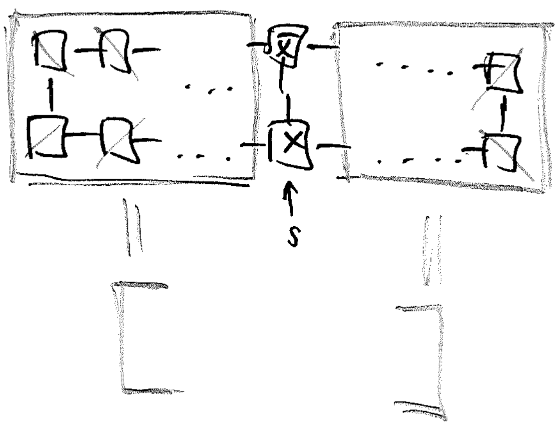
$\Rightarrow$ find X s.th. $E[X]$ is minimal! (*)

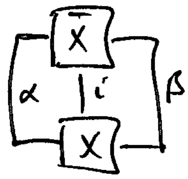
Replace $A^{[s]}$ by X!

3. Iterate Step 2 over all lattice sites back and forth (i.e.: $s = 1, 2, \dots, N-1, N, N-1, \dots, 2, 1, 2, 3, \dots$, etc.), until the energy converges.

Remains to show: How can we solve the minimization problem (*)?

1. Choose isometric gauge around site s:

$\langle\psi[X]|\psi[X]\rangle =$ 

$=$ 

$= \sum_{\alpha\beta i} \bar{X}^i_{\alpha\beta} X^i_{\alpha\beta} = \vec{X}\cdot\vec{X}$,

if we interpret $X^i_{\alpha\beta} \equiv \vec{X}$ as a vector.

⇒ We need to solve

$$\min_{\vec{X}\cdot\vec{X}=1} \langle\psi[X]|H|\psi[X]\rangle$$

2. $|\psi[X]\rangle = \sum \mathrm{tr}[A^{[1]i_1} \cdots X^{i_s} \cdots A^{[N]i_N}]\,|i_1,\dots,i_N\rangle$

is linear in X!

$\Rightarrow \langle\psi[X]|H|\psi[X]\rangle = \vec{x}\cdot M\vec{x}$ is a quadratic form in $\vec{x}$!, $M = M^\dagger$

$$\min_{|\vec{x}|_2=1} \vec{x}\cdot M\vec{x}$$

↑ equals the smallest eigenvalue of M; λ_{min}

and the optimal $\vec{x}$ is the eigenvector

$$M\vec{x} = \lambda_{min}\vec{x}$$

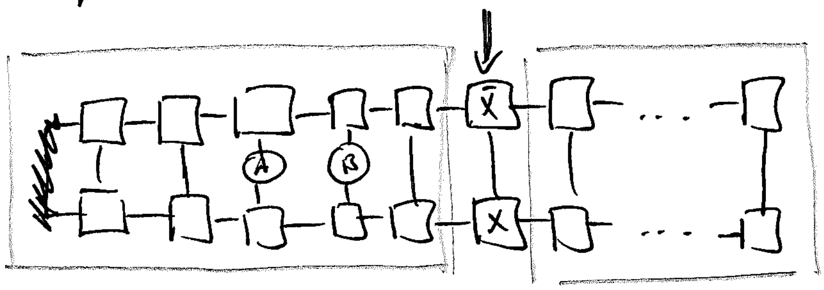
⇒ once we know M, we only need to solve an eigenvalue problem!

So how can we compute M?

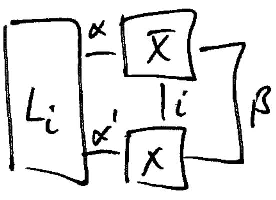
restrict to $h_i = A_i \otimes B_{i+1}$

$$\langle\psi[x]|H|\psi[x]\rangle = \sum_i \underbrace{\langle\psi[x]|h_i|\psi[x]\rangle} \equiv \vec{x}\cdot M_i\vec{x}$$

<u>two types of terms:</u>

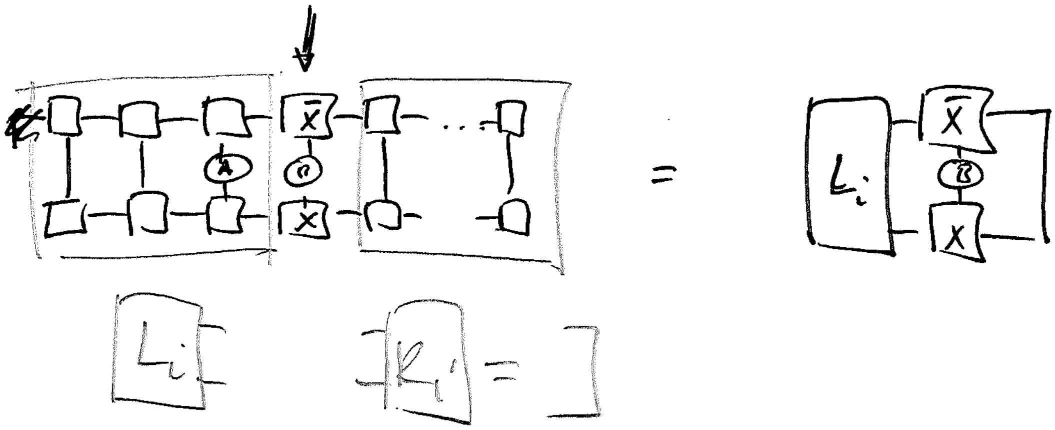


(isometric Gauge!)

=  ⇒ leads to $M_i = \mathbb{1} \otimes (L_i) \otimes \mathbb{1}$

$i \qquad \alpha,\alpha' \qquad \beta$

Other term:



$$\Rightarrow \quad M_i = \underset{i,i'}{B} \otimes \underset{\alpha,\alpha'}{(L_i)} \otimes \underset{\beta}{\mathbb{1}}$$

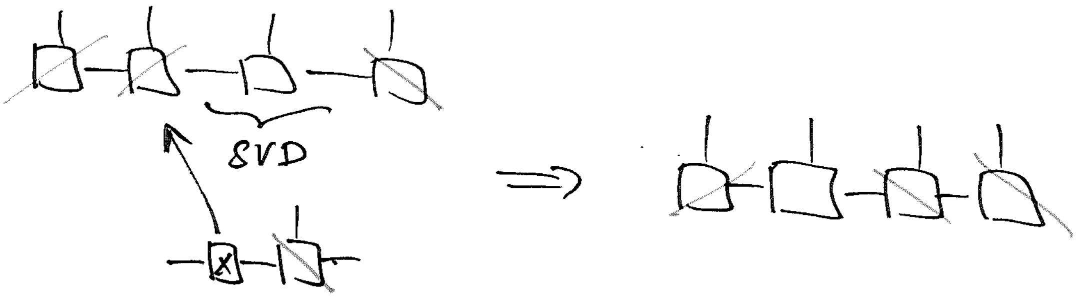
$$\Rightarrow \quad M = \sum M_i \text{ over \underline{all Ham. terms}}$$

~~Simplification for a more efficient algorithm:~~

- ~~Iso. gauge can be moved from s → s+1 by one local update.~~
- ~~L_i and R_i (for $i \leq s$)~~
- ~~L_i can be updated easily when moving to the right. (and correspondingly for R_i when moving left)~~
- ~~For all terms left of a given cut s, we only need to keep $\sum_{i<s} L_i[s] = L[s]$~~

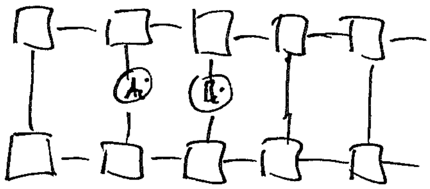
Simplification for more efficient algorithm:

- Iso. gauge w/ center s can be moved to $s+1$ (or $s-1$) w/ a local update



- The whole influence of all Ham. terms left (or right) of a cut s can be summarized in

$$L[s] = \sum_{\substack{A_i \otimes B_{i+1} \\ \text{left of } s}}$$



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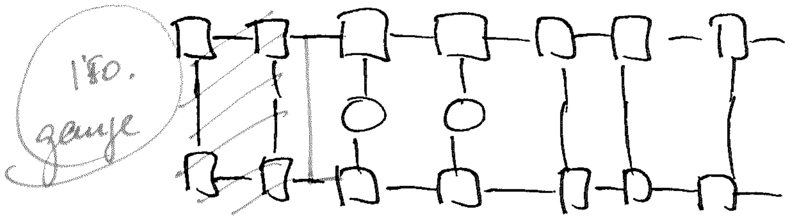
- $L[s]$ can updated locally when moving $s \to s+1$. (We just have to add new terms and can use iso. gauge.)
- If we store $L[k]$ for all $k \leq s$ (the cut), then we can also move $s \to s-1$ w/out any computation.
- Corresp. for the right!

Improved contraction scaling in D:

To compute



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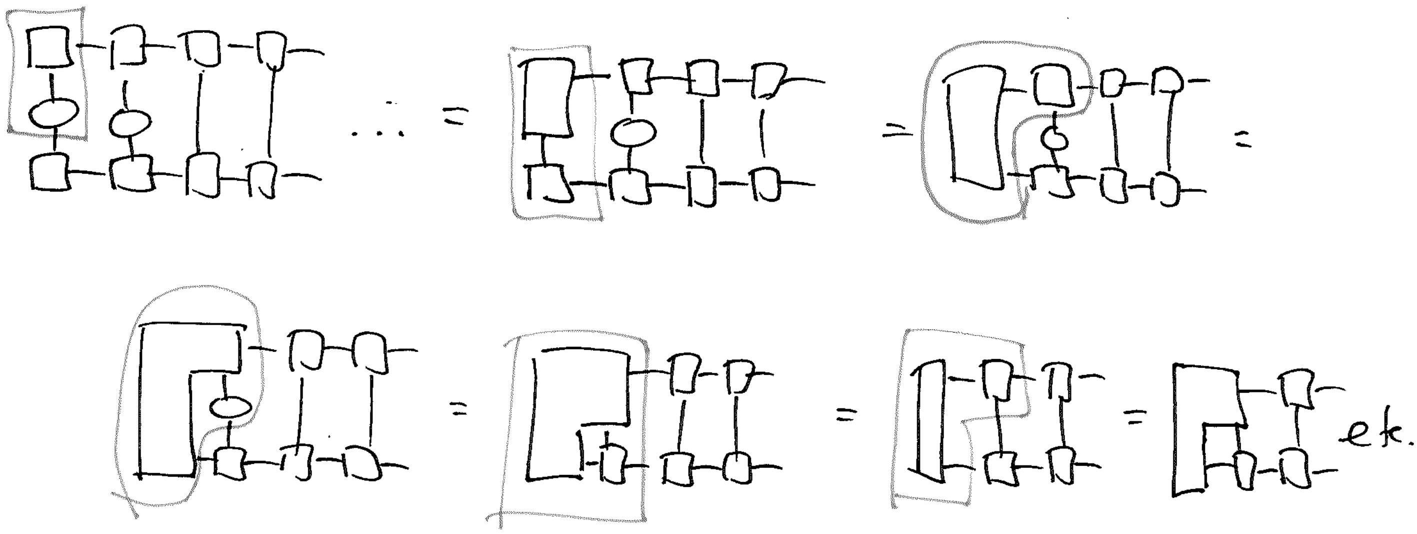
contract as follows:



At most mult. of ~~dD~~ $D\times(dD)$ matrix w/ $(dD)\times D$ matrix necessary

$\rightarrow$ scales as ~~…~~ $dD^3 \ll D^4$ for large D!