

# Introduction to Matrix Product States (MPS)

Motivation: analytic solutions for interacting systems are often approximations  
 → quantitative predictions are hard

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- Outline : 1) Intro to tensor networks  
 2) MPStates 3) MPOperators  
 4) gradient-based variational algorithms
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## 1) Intro to tensor networks

$T_{i_1 i_2 \dots j_1 j_2 \dots}$  { Proper definition: multilinear map of a certain type  
 For our purposes here: just think of some multidimensional array

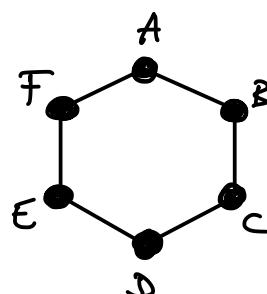
Examples: scalar  $\hat{=}$   $s \hat{=}$   $\bullet$   
 vector  $\hat{=}$   $\{v_i\} \hat{=}$   $\text{↑}$   
 matrix  $\hat{=}$   $\{m_{ij}\} \hat{=}$   $- \bullet -$   
 $\vdots$

Each index has a "dimension"  $\hat{=}$  #elements

use graphical notation to simplify tensor contractions !

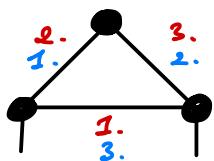
$$A_{ij} B_{ik} = i \sum_j \bullet \overset{j}{\bullet} \bullet k = i \bullet k$$

$$A_{ij} B_{jk} C_{kl} D_{lm} E_{mn} F_{ni} = \text{tr}(ABCDEF)$$



Order of contractions  $\xrightarrow{\text{linked to}}$  complexity class

Example:



assume the dimension of all indices to be  $D$

$$1. \hat{=} \Theta(D^5), \text{ result:}$$

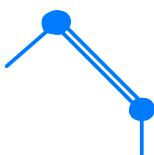


$$2.+3. \hat{=} \Theta(D^4)$$

in total: complexity class  $\Theta(D^5)$

in contrast:

$$1. \hat{=} \Theta(D^4), \text{ result:}$$



$$2.+3. \hat{=} \Theta(D^4)$$

\* preferred sequence!

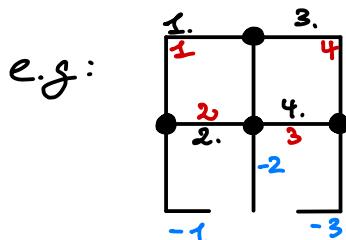
Steps to perform contractions (numerically):

1. fix index order of all tensors (common notation: negative numbers)

e.g.:

$\rightarrow$  we use these objects later ...

2. define "links" and "open" indices and  
define the order of the contraction sequence



(common notation: positive numbers)

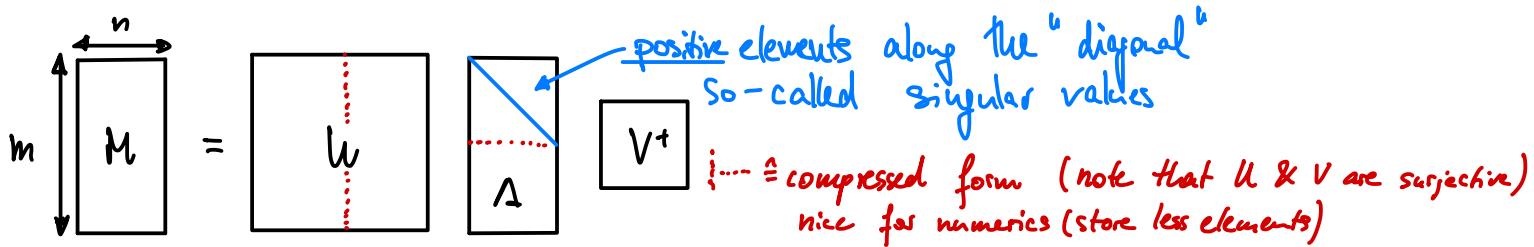
(common notation: negative numbers)

# Singular Value Decomposition (SVD)

The SVD decomposes a matrix into a rotation, a coordinate scaling, and another rotation.

$$M = U \Lambda V^+ \text{ with } U^T U = V^T V = I$$

Suppose  $M$  is  $m \times n$ , then  $U$  is  $m \times m$ ,  $\Lambda$  is  $m \times n$  &  $V^+$  is  $n \times n$ .



- the SVD is not unique, the nonzero elements of  $\Lambda$  are, though.
- $U$  &  $V$  are matrices composed of basis vectors

$$M^T M = V \Lambda^* U^T U \Lambda V^+ = V (\Lambda^* \Lambda) V^+$$

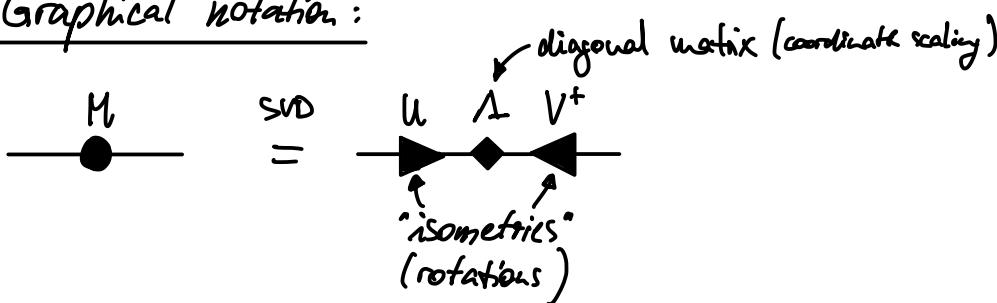
$$M M^T = U \Lambda V^+ V \Lambda^* U^T = U (\Lambda \Lambda^*) U^T$$

$\Rightarrow$  the columns of  $V/U$  are the eigenvectors of  $M^T M / M M^T$ .

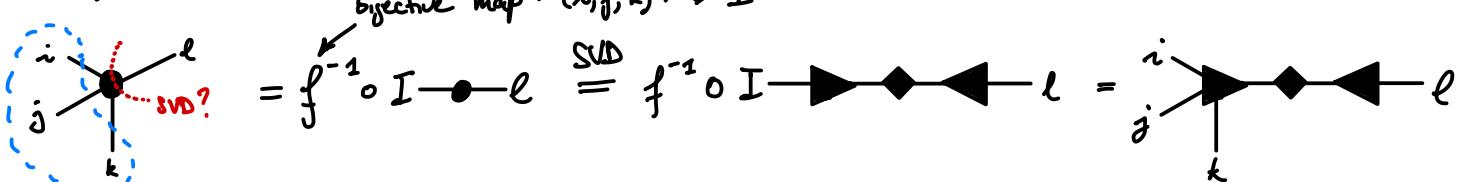
- $M$  normal ( $M = AA^*$ )  $\xrightarrow[\text{spectral theorem}]{\Rightarrow} M = U D U^+$  with unitary  $U$  & diagonal  $D$ . If  $M \geq 0$ , then  $D \geq 0$  and  $D = \Lambda$ .

many applications: pseudoinverse, solving linear eq's, least squares minimization, ...

## Graphical notation:



Generalization:



## 2) Matrix Product States (MPS)

Consider a generic many-body state formed by  $L$ -constituents that each have a local Hilbert space  $\mathcal{H}_i = \text{span} \{ |i\rangle, i=1, \dots, d\}$   
 (e.g.  $|0\rangle = |\uparrow\rangle$  and  $|1\rangle = |\downarrow\rangle$  for spin- $\frac{1}{2}$ 's)

$$|\Psi\rangle = \sum_{i_1, i_2, \dots, i_L} C(i_1, i_2, \dots, i_L) |i_1, i_2, \dots, i_L\rangle$$

$$C: N^L \rightarrow \mathbb{C}, \Rightarrow \{C(i)\} \sim d^L \text{ complex numbers}$$

Can we find a "better" representation?

$$C(i_1) = \begin{array}{c} i_2 \\ \vdots \\ i_1 \\ \vdots \\ i_2 \\ \vdots \\ i_3 \\ \vdots \\ i_4 \end{array} = \begin{array}{c} \boxed{\phantom{0}} \\ \vdots \\ \boxed{\phantom{0}} \\ \vdots \\ \boxed{\phantom{0}} \\ \vdots \\ \boxed{\phantom{0}} \end{array} = f^{-1} \circ i_1 \bullet I_2$$

$$\stackrel{\text{SVD}}{=} f^{-1} \circ i_1 \xrightarrow{\quad} \begin{array}{c} \blacktriangleleft \\ \blacktriangleright \end{array} \xrightarrow{\quad} I = i_1 \xrightarrow{\quad} \begin{array}{c} \boxed{\phantom{0}} \\ \vdots \\ \boxed{\phantom{0}} \end{array} = \tilde{f}^{-1} \circ I \bullet i_1$$

$$\stackrel{\text{SVD}}{=} \tilde{f}^{-1} \circ \begin{array}{c} \tilde{I} \\ \xrightarrow{\quad} \end{array} \begin{array}{c} \blacktriangleleft \\ \blacktriangleright \end{array} i_L = i_1 \xrightarrow{\quad} \begin{array}{c} \boxed{\phantom{0}} \\ \vdots \\ \boxed{\phantom{0}} \end{array} \xleftarrow{\quad} i_L = \tilde{f}^{-1} \circ i_2 \xrightarrow{\quad} \begin{array}{c} \tilde{I} \\ \xrightarrow{\quad} \end{array}$$

$$\stackrel{\text{SVD}}{=} \tilde{f}^{-1} \circ i_2 \xrightarrow{\quad} \begin{array}{c} \blacktriangleleft \\ \blacktriangleright \end{array} \xrightarrow{\quad} \begin{array}{c} \tilde{I} \\ \xrightarrow{\quad} \end{array} = i_1 \xrightarrow{\quad} \begin{array}{c} \boxed{\phantom{0}} \\ \vdots \\ \boxed{\phantom{0}} \end{array} \xrightarrow{\quad} i_L$$

⋮ repeat

$$= \begin{array}{ccccccccccccc} \xrightarrow{\quad} & \xrightarrow{\quad} & \xrightarrow{\quad} & \xrightarrow{\quad} & \cdots & \xrightarrow{\quad} & \blacktriangleleft & \xrightarrow{\quad} & \cdots & \xrightarrow{\quad} & \blacktriangleleft & \xrightarrow{\quad} & \cdots & \xrightarrow{\quad} & \blacktriangleleft & \xrightarrow{\quad} \\ i_1 & i_2 & i_3 & i_4 & & i_l & i_{l+1} & i_{l-1} & & i_{l-3} & i_{l-2} & i_{l-1} & & i_l & & & \end{array}$$

$U^{[i_2]} \quad A(l) = \begin{pmatrix} s_1 & \theta \\ 0 & s_{l-1} \end{pmatrix} \quad V^{[i_{l-1}]}$

$$= \left( \prod_{k=1}^l U^{[i_k]} \right) A(l) \left( \prod_{k=l+1}^L V^{[i_k]} \right)$$

Why scalar?

→  $U^{[i_2]}, V^{[i_l]}$  are vectors

for fixed  $i_2, i_l$

$$\begin{aligned}
|\Psi\rangle &= \sum_{i_1} C(i_1, i_2, \dots, i_L) |i_1, i_2, \dots, i_L\rangle \quad \text{this is exact} \\
&= \sum_i \begin{array}{ccccccc} \nearrow & \nearrow & \cdots & \nearrow & \nearrow & \cdots & \nearrow \\ i_1 & i_2 & & i_e & i_{e+1} & & i_L \end{array} |i_1, i_2, \dots, i_L\rangle \\
&= \sum_i \left( \frac{\ell}{\prod_{k=1}^L} u^{[i_k]} \right) \Lambda(\ell) \left( \prod_{k=e+1}^L V^{[i_k]} \right) |i_1, i_2, \dots, i_L\rangle \\
&\quad \Lambda_{mn} = S_m \delta_{mn} \\
&= \sum_{m,n} \sum_i \left( \frac{\ell}{\prod_{k=1}^L} u^{[i_k]} \right)_m \Lambda(\ell)_{mn} \left( \prod_{k=e+1}^L V^{[i_k]} \right)_n |i_1, i_2, \dots, i_L\rangle \\
&= \sum_m \sum_i \left( \frac{\ell}{\prod_{k=1}^L} u^{[i_k]} \right)_m S_m(\ell) \left( \prod_{k=e+1}^L V^{[i_k]} \right)_m |i_1, i_2, \dots, i_L\rangle \\
&= \underbrace{\sum_m \left( \sum_{i_1, \dots, i_e} \left( \frac{\ell}{\prod_{k=1}^L} u^{[i_k]} \right)_m |i_1, i_2, \dots, i_e\rangle \right) S_m(\ell)}_{|\Psi_{A(\ell), m}\rangle} \underbrace{\left( \sum_{i_{e+1}, \dots, i_L} \left( \prod_{k=e+1}^L V^{[i_k]} \right)_m |i_{e+1}, i_{e+2}, \dots, i_L\rangle \right)}_{|\Psi_{B(\ell), m}\rangle} \\
&= \sum_m S_m(\ell) \underbrace{|\Psi_{A(\ell), m}\rangle}_{\in \mathcal{H}_A} \underbrace{|\Psi_{B(\ell), m}\rangle}_{\text{product state}} \quad \text{"Schmidt-decomposition"} \\
\end{aligned}$$

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Reduced density matrix

$$A \cup B = L, \quad B = A^c$$

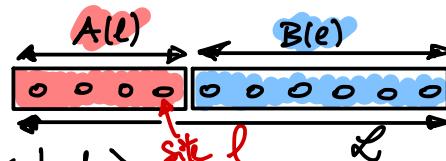
$$\hat{\rho}_A = \text{tr}_B \hat{\rho} = \sum_{\{\phi_B\}} \langle \phi_B | \Psi \rangle \langle \Psi | \phi_B \rangle$$

↓  
 orthonormal basis  
 of vectorspace  $\mathcal{H}_B$

$$= \sum_n \langle \phi_{B,n} | \left( \sum_m S_m(\ell) |\Psi_{A'(\ell), m}\rangle \langle \Psi_{B'(\ell), m}| \right) \left( \sum_{m'} S_{m'}^*(\ell) \langle \Psi_{A'(\ell), m'} | \langle \Psi_{B'(\ell), m'} | \right) | \phi_{B,n} \rangle$$

1. choose  $\ell$  such that  $B'(\ell) = B$  (always possible in 1D)
2.  $|\Psi_{B,m}\rangle = U_{mj} |\phi_{B,j}\rangle$  rotate  $\Psi$  to  $\phi$

## Reduced density matrix



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↑ orthonormal basis  
of vectorspace  $\mathcal{H}_B$

$$= \sum_n \langle \phi_{B,n} | \left( \sum_m S_m(l) |\psi_{A'(l),m}\rangle \langle \psi_{B'(l),m}| \right) \left( \sum_{m'} S_{m'}^*(l) \langle \psi_{A'(l),m'} | \langle \psi_{B'(l),m'} | \right) | \phi_{B,n} \rangle$$

1. choose  $\tilde{l}$  such that  $B'(\tilde{l}) = B$  (always possible in 1D)

2.  $|\psi_{B,m}\rangle = U_{mj} |\phi_{B,j}\rangle$  rotate  $\Psi$  to  $\phi$

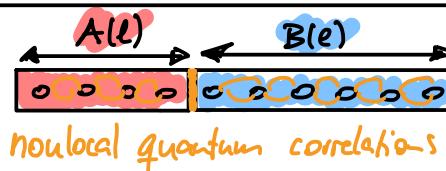
$$= S_m(\tilde{l}) S_{m'}^*(\tilde{l}) U_{mj} U_{m'j'}^* \underbrace{\langle \phi_{B,n} | \phi_{B,j} \rangle}_{\delta_{nj}} \underbrace{\chi \langle \phi_{B,j'} | \phi_{B,n'} \rangle}_{\delta_{n'j'}} |\psi_{A,m} \rangle \langle \psi_{A,m'}|$$

$$= S_m(\tilde{l}) S_{m'}^*(\tilde{l}) \underbrace{U_{mj} U_{m'j'}}_{\delta_{mm'}} |\psi_{A,m} \rangle \langle \psi_{A,m'}|$$

$$= \sum_m |S_m(\tilde{l})|^2 |\psi_{A,m} \rangle \langle \psi_{A,m'}|$$

thermal density matrix operator  
(it's diagonal in  $\mathcal{H}_A$ )

## Entanglement entropies



$$S_1(l) = - \text{tr} \hat{\rho}_{A(l)} \ln \hat{\rho}_{A(l)} = - \sum_m |S_m(l)|^2 \ln |S_m(l)|^2$$

$$= - \text{tr} |\Lambda(l)|^2 \ln |\Lambda(l)|^2$$

↳ once in MPS-form,  $S_1(l)$  is directly accessible!

$$\max S_1(l) = - \text{tr} \hat{\rho}_{\infty} \ln \hat{\rho}_{\infty} = - \sum_{m=1}^X X^{-1} \ln X^{-1} = + \ln X \quad || \quad \begin{array}{l} \text{(extensive)} \\ \text{"infinite temperature"} (\hat{\rho}_{\infty})_{ij} = X^{-1} \delta_{ij}, X = \dim \mathcal{H}_{A(l)} \end{array} \quad || \quad \begin{array}{l} \text{upper bound given by} \\ \text{the dimension of } \mathcal{H}_{A(l)} \end{array}$$

$S_1$  is called von Neumann entropy and the special case of the more general Rényi entropy (inspired from quantum info-Shannon entropy)

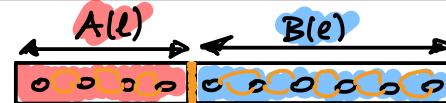
$$S_\alpha(l) = \frac{1}{\alpha-1} \ln \text{tr} \hat{\rho}_A^\alpha$$

Gives entropy from microstates distribution

$$S = -k_B \sum_i p_i \ln p_i$$

↑ microstate probability

## Entanglement entropies



nonlocal quantum correlations

$$S_1(l) = -\text{tr} |\Lambda(l)|^2 \ln |\Lambda(l)|^2 \quad \max S_1(l) = +\ln N$$

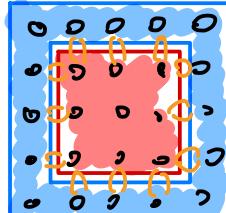
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$$S_\alpha(l) = \frac{1}{\alpha-1} \ln \text{tr} \hat{\rho}_A^\alpha$$

- $N$ -partite separability criterion (i.e. can I find a Schmidt decomposition s.t.  $\text{Im}, S_m = 1$ )
  - is the state I'm having here a product state in the bipartitions A/B?
- $S_1 = 0 \Leftrightarrow$  state is  $N$ -partite separable.
- The low-energy states of gapped Hamiltonians often respect an "area law"
 
$$S_1(l) \sim \mathcal{L}(l) \leftarrow \text{area between the bipartition A/B}$$

e.g.  $D=1$  :   $S_1(l) \sim \text{const}$

$D=2$  :   $S_1(l) \sim l$

$D=1$  Hastings, 2007  
(only SPTP Phases with "trivial" topological order)

$D > 1$  very complicated business  
(J. Eisert, X-G Wen & many others)

MPS respect the 1D area law  $\rightarrow$  efficient representation of low-energy manifold

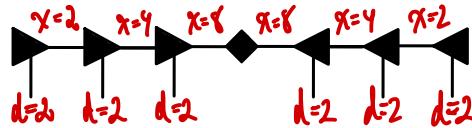
$$S_1 = -\text{tr} \Lambda^2 \ln \Lambda^2$$

$$|\Psi\rangle = \sum_i \begin{array}{ccccccc} \nearrow & \nearrow & \cdots & \nearrow & \nearrow & \cdots & \nearrow \\ i_1 & i_2 & & i_r & i_{r+1} & & i_s \end{array} |i_1, i_2, \dots, i_s\rangle$$

## Compression of generic many body states

- $\dim \Lambda = \min(\dim(\mathcal{H}_A), \dim(\mathcal{H}_B))$

Example: MPS of Spin $\frac{1}{2}$  chain



- $S_1^{(l)} = -\text{tr} \Lambda^2(l) \ln \Lambda^2(l)$ , 1D area law:  $S_1 = \text{const.}$

$$\Rightarrow \forall l \exists X < \infty \text{ s.t. } |\Psi\rangle = \sum_{m=1}^X S_m^{(l)} |\Psi_{A(l), m}\rangle |\Psi_{B(l), m}\rangle$$

» this implies that 1D area law states have a finite number of  $\{S_m(l)\}$ , even  $\ll$  in the thermodynamic limit

- arbitrary states: (i) fix  $X \in \mathbb{N}$

(ii) keep only the  $X$  largest  $\{S_m(l)\}$   $\forall l$

(iii) renormalize to  $\sum S_m^2(l) = 1 \quad \forall l$

→ you'll get  $|\Psi'\rangle$  s.t.  $S_1^{(\Psi')}(l) \approx S_1^{(\Psi)}(l)$ , the precision of the approximation is controlled by  $X$

## 3) Matrix Product Operators (MPO)

Example: local operator on site  $q$ ,  $\hat{O}_q = \sum_{i_1, i_2, \dots, i_q} O_{i_1, i_2, \dots, i_q} |i_1 i_2 \dots i_q|$

Action on generic MPS:

$$\begin{aligned}
 \hat{O}_q |\Psi\rangle &= \hat{O}_q \sum_i C(i) |i_1, i_2, \dots, i_q, \dots, i_l\rangle \\
 &= \sum_{i_1, i_2} O_{i_1, i_2} \sum_i C(i) |i_1, \dots, i_{q-1}\rangle |i_q \underbrace{i_q''}_{i_q} |i_q\rangle |i_{q+1}, \dots, i_l\rangle \\
 &= \sum_{i_1} \sum_{i_2} O_{i_1, i_2} C(i) |i_1, \dots, i_{q-1}, i'_q, i_{q+1}, \dots, i_l\rangle \\
 &= \sum_i \tilde{C}(i) |i\rangle
 \end{aligned}$$

*embed  $\sum_{i_1}$ , rename  $i_2 \rightarrow i_1$        $S_{i_1, i_2}$*

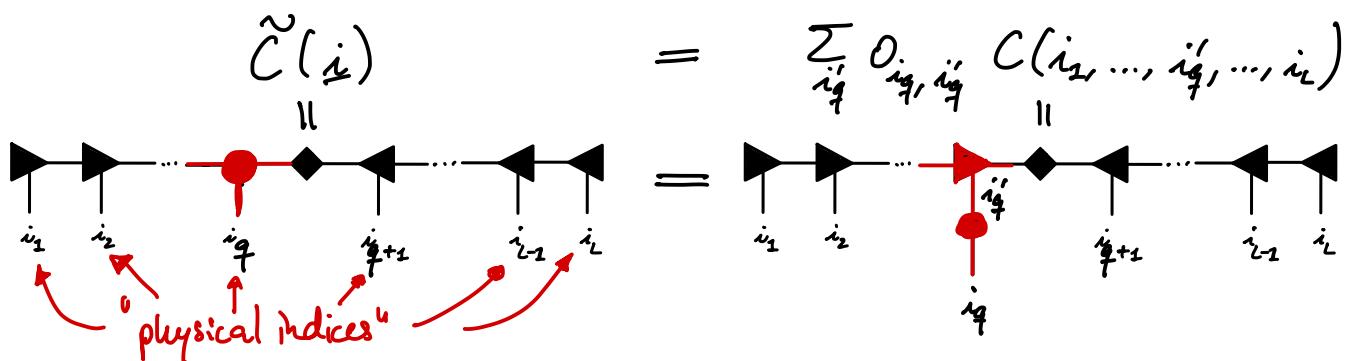
$$\tilde{C}(i) = \sum_{i_1} O_{i_1, i_2} C(i_1, \dots, i'_q, \dots, i_l)$$

### 3) Matrix Product Operators (MPO)

Example: local operator on site  $q$ ,  $\hat{O}_q = \sum_{i_1, i_2} O_{i_1, i_2, q} |i_1 i_2 \dots q \dots i_2 i_1\rangle$

Action on generic MPS:

$$\begin{aligned}\hat{O}_q |\Psi\rangle &= \hat{O}_q \sum_i C(i) |i_1, i_2, \dots, i_q, \dots, i_n\rangle \\ &= \sum_i \tilde{C}(i) |i\rangle\end{aligned}$$



⇒ local operators transform the local matrices of the MPS by a contraction of the physical index

This allows to reformulate any Hamiltonian composed of (local) operators in terms of a so-called "MPO"

### Ising model

$$\hat{H} = \hat{H}_h + \hat{H}_J, \quad \hat{H}_J = J \sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x, \quad \hat{H}_h = h \sum_i \hat{\sigma}_i^z$$

↑  
ordering of nearest neighbors:  $J \geq 0$  parallel, e.g.  $\uparrow\uparrow$   
anti-parallel, e.g.  $\uparrow\downarrow$

external field along z-axis

## Ishy model

$$\hat{H} = \hat{H}_h + \hat{H}_J \quad , \quad \hat{H}_J = J \sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x \quad , \quad \hat{H}_h = h \sum_i \hat{\sigma}_i^z$$

$$\hat{H} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddots & \hat{W}_i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$$

**MPO!**

with  $\hat{W}_i = \begin{pmatrix} \hat{\sigma}_i^z & \hat{\sigma}_i^x & h\hat{\sigma}_i^z \\ 0 & 0 & \hat{\sigma}_i^x \\ 0 & 0 & \hat{\sigma}_i^z \end{pmatrix}$

Check for  $L=3$ :

$$\begin{pmatrix} 1 & x_1 & h_2 \\ 0 & 0 & \cancel{fx_1} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & x_2 & h_2 \\ 0 & 0 & \cancel{fx_2} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & x_3 & h_2 \\ 0 & 0 & \cancel{fx_2} \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & x_2 & h_2 \\ 0 & 0 & \cancel{fx_1} \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & x_3 & h_2 \\ 0 & 0 & \cancel{fx_3} \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & x_3 & h_2 \\ 0 & 0 & \cancel{fx_1} \\ 0 & 0 & 1 \end{pmatrix}$$

$$H_2 = [h^2_2 + f x_1 x_2 + h^2_1] \quad H_3 = [h^2_3 + f x_2 x_3 + h^2_2 + f x_1 x_2 + h^2_1]$$

$$\Rightarrow \prod_{i=1}^L \hat{W}_i = \begin{pmatrix} \hat{I}_L & \hat{\sigma}_L & \hat{H}_L \\ 0 & 0 & \hat{J}\hat{\sigma}_L \\ 0 & 0 & \hat{I}_L \end{pmatrix} \Rightarrow \hat{H} = (1 \ 0 \ 0) \begin{pmatrix} \hat{I}_L & \hat{\sigma}_L & \hat{H}_L \\ 0 & 0 & \hat{J}\hat{\sigma}_L \\ 0 & 0 & \hat{I}_L \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = (1 \ \hat{\sigma}_L \ \hat{H}_L) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hat{H}_L \quad \checkmark$$

## Graphical notation

$$\hat{W}_q = \left\{ (W_q^{lm})_{i_1^q, i_2^q} \mid i_1^q \in \chi_{i_1^q}, i_2^q \in \chi_{i_2^q} \right\}_{l,m} = \left\{ l - \begin{array}{c} i_1^q \\ i_2^q \end{array} m \right\}_{l,m}$$

$$\hat{H} = \sum_{\underline{i}''} \sum_{\underline{i}'} | \underline{i}' \chi \underline{i}'' |$$

## Energy expectation value

$$\langle \Psi | \hat{H} | \Psi \rangle = \text{Diagram showing a 2D grid of qubits with various interactions (dots, diamonds, triangles) between them. The right side is annotated with red text: } \} \stackrel{\wedge}{=} C(i) \text{ and } \} \stackrel{\wedge}{=} C^*(i')$$

## Gradient based algorithms

- variational principle: minimize  $E(\Psi) = \langle \Psi | H | \Psi \rangle$ ,  $\langle \Psi | \Psi \rangle = 1$   
 Using lagrange multiplier, we can recast this to  

$$\mathcal{L} = \langle \Psi | H | \Psi \rangle - \lambda (\langle \Psi | \Psi \rangle - 1)$$

This variation  $\delta \mathcal{L} = 0$  yields equations of motion for the vectors  $\{\langle \Psi |, |\Psi \rangle\}$  that satisfy the Schrödinger equation

$$0 = \frac{\partial \mathcal{L}}{\partial \langle \Psi |} - \partial_t \frac{\partial \mathcal{L}}{\partial |\Psi \rangle} = H |\Psi \rangle - \lambda |\Psi \rangle \Rightarrow H |\Psi \rangle = \lambda |\Psi \rangle$$

We now exploit the internal matrix product structure of  $|\Psi \rangle$  in order to obtain local instead of global com's.  
 Let's switch to the graphical notation, using the building blocks:

$$\begin{aligned} \langle \Psi | \hat{H} | \Psi \rangle &= \text{Diagram showing a horizontal chain of nodes connected by arrows pointing right, with a central node connected to two others.} \\ \langle \Psi | \Psi \rangle &= \text{Diagram showing a horizontal chain of nodes connected by arrows pointing right, with a central node connected to two others.} \\ \Rightarrow \mathcal{L} &= \text{Diagram showing a horizontal chain of nodes connected by arrows pointing right, with a central node connected to two others.} - \lambda \left( \text{Diagram showing a horizontal chain of nodes connected by arrows pointing right, with a central node connected to two others.} - 1 \right) \end{aligned}$$

Since the Lagrangian does not contain total time derivatives,  
 the variational principle applied to the central tensor  $T = \text{Diagram}$

$$0 = \frac{\delta \mathcal{L}}{\delta T} = \left\{ \frac{\partial \mathcal{L}}{\partial (T_{m,i_e, i_{e+1}, n})} \right\}_{i_e, i_{e+1}, m, n}$$

is simply a gradient w.r.t. the tensor elements  $T_{m,i_e, i_{e+1}}$ .

Furthermore,  $\mathcal{L}$  is linear in  $T$ , such that the gradient graphically amounts to just erasing  $T$  in the picture.

## Gradient based algorithms

- variational principle:  $\mathcal{L} = \langle \Psi | H | \Psi \rangle - \lambda (\langle \Psi | \Psi \rangle - 1)$

$$\mathcal{L} = \begin{array}{c} \text{Diagram of } \langle \Psi | H | \Psi \rangle \\ \text{with red arrows indicating flow from left to right} \end{array} - \lambda \left( \begin{array}{c} \text{Diagram of } \langle \Psi | \Psi \rangle \\ \text{with red arrows indicating flow from left to right} \end{array} - 1 \right)$$

$$O \stackrel{!}{=} \frac{\delta \mathcal{L}}{\delta \psi_{i_e, i_{e+1}, m, n}} = \left\{ \frac{\partial \mathcal{L}}{\partial (\psi_{i_e, i_{e+1}, m, n})} \right\}_{i_e, i_{e+1}, m, n}$$

$\Leftrightarrow$

$$\begin{array}{c} \text{Diagram of } \langle \Psi | H | \Psi \rangle \\ \text{with red arrows indicating flow from left to right} \end{array} = \lambda \begin{array}{c} \text{Diagram of } \langle \Psi | \Psi \rangle \\ \text{with red arrows indicating flow from left to right} \\ \text{with curved arrows labeled "unitaries"} \end{array}$$

$\Leftrightarrow$

$$\begin{array}{c} \text{Diagram of } \langle \Psi | H | \Psi \rangle \\ \text{with blue arrows indicating flow from left to right} \end{array} = \lambda \begin{array}{c} \text{Diagram of } \langle \Psi | \Psi \rangle \\ \text{with blue arrows indicating flow from left to right} \end{array}$$

let's reshape the blue object to a vector, i.e.

$$f \circ \psi_{i_1, i_2, i_3, i_4} = I \bullet$$

and the black object to a matrix, i.e.

$$g \circ \begin{array}{c} \text{Diagram of } \langle \Psi | \Psi \rangle \\ \text{with black arrows indicating flow from left to right} \end{array} = I' \bullet I$$

then we obtain a simple eigenvector problem:

$$\bullet \bullet = A \bullet$$

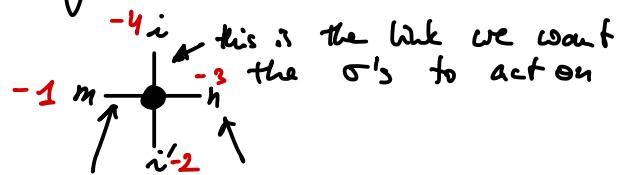
This can be implemented efficiently and then passed to a sparse eigenvalue solver (e.g. ARPACK-package).

hands-on!

→ DMRG, VUMPS, **iDMRG**, TDVP, ... ←

Implement the MPO of  $H$

$$W = \begin{pmatrix} 1 & \sigma^x & h\sigma^z \\ 0 & 0 & 3\sigma^x \\ 0 & 0 & 1 \end{pmatrix}$$



this is the link to obtain  $H$  as  
a contraction of all  $W$ 's

$$W = \begin{pmatrix} W_{m,i} & \downarrow & \downarrow \\ \uparrow & \dim=2 \\ W_{m,i'} & n_i \end{pmatrix}$$

$\dim=3$

$$L = [1 \ 0 \ 0] \quad \left( \equiv \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \right)$$

$$R = [0; \ 0; \ 1;] \quad \left( \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right)$$

Check your construction for small system size

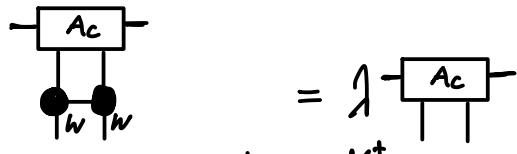
$$LWWR \equiv J\sigma_x \otimes \sigma_x + h\sigma_z \otimes 1 + h1 \otimes \sigma_z$$

$$LWWWR = J(\sigma_x \otimes \sigma_x \otimes 1 + 1 \otimes \sigma_x \otimes \sigma_x) + h(\sigma_z \otimes 1 \otimes 1 + 1 \otimes \sigma_z \otimes 1 + 1 \otimes 1 \otimes \sigma_z)$$

$$LWWWWWR = \dots$$

## iDMRG

- choose  $n$  ( $= \frac{L}{2}$  with  $L$  even). This is your number of iterations
- $i = 1$ : compute the lowest energy  $A_C^{[i_1, i_2]}$  for a system of 2 sites



$$3. \text{ SVD: } \boxed{\quad} = \underset{U}{\leftarrow} \underset{\Lambda}{\downarrow} \underset{V^+}{\rightarrow}$$

$$4. \text{ Grow: } \cdots \leftarrow \underset{U}{\leftarrow} \underset{\Lambda}{\downarrow} \underset{V^+}{\rightarrow} \cdots \longrightarrow \cdots \leftarrow \underset{U}{\leftarrow} \underset{A_C^i}{\downarrow} \underset{V^+}{\rightarrow} \cdots, \quad i = i + 1$$

$$5. \text{ Lowest energy } A_C: \quad \boxed{\quad} = \underset{U}{\leftarrow} \underset{\Lambda}{\downarrow} \underset{V^+}{\rightarrow} \boxed{\quad}$$

6. if  $i < n \rightarrow 3.$

↳ from final  $A_C$ , compute observables