

Introduction to Matrix Product States (MPS)

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

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

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

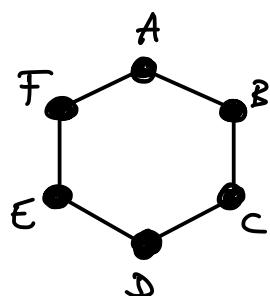
Examples: scalar $\hat{=}$ $s \hat{=}$ \bullet
 vector $\hat{=}$ $\{v_i\} \hat{=}$ ↑
 matrix $\hat{=}$ $\{m_{ij}\} \hat{=}$ $- \bullet -$
 \vdots

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

use graphical notation to simplify tensor contractions !

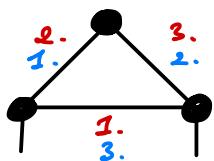
$$A_{ij} B_{ik} = i \sum_j \bullet \overset{j}{\bullet} \bullet k = i \bullet k$$

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



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

Example:



assume the dimension of all indices to be D

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

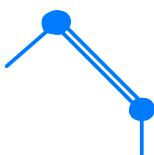


$$2.+3. \hat{=} \Theta(D^4)$$

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

in contrast:

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



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

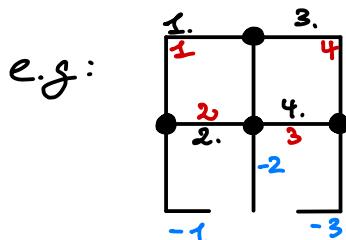
* preferred sequence!

Steps to perform contractions (numerically):

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

e.g.:

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



(common notation: positive numbers)

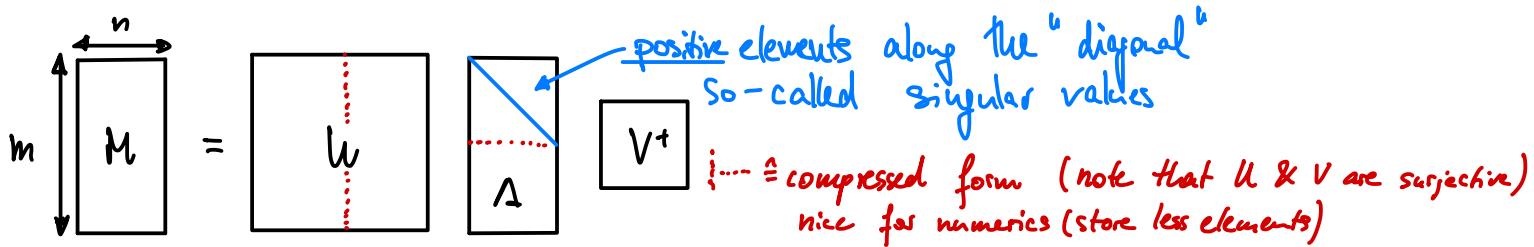
(common notation: negative numbers)

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 $m \times m$, Λ is $m \times n$ & V^+ is $n \times n$.



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

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

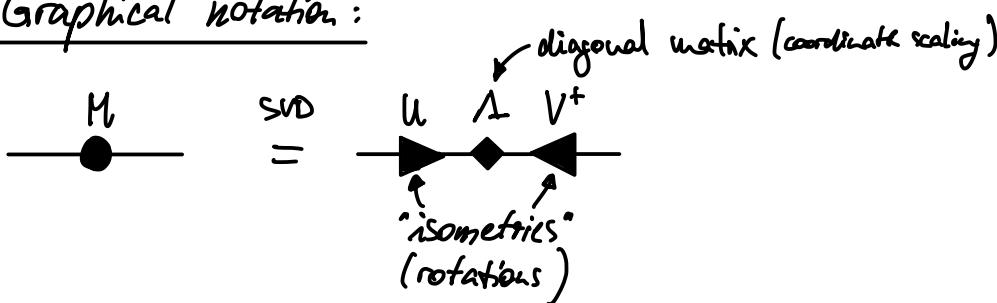
$$M M^T = U \Lambda V^+ V \Lambda^* U^T = U (\Lambda \Lambda^*) U^T$$

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

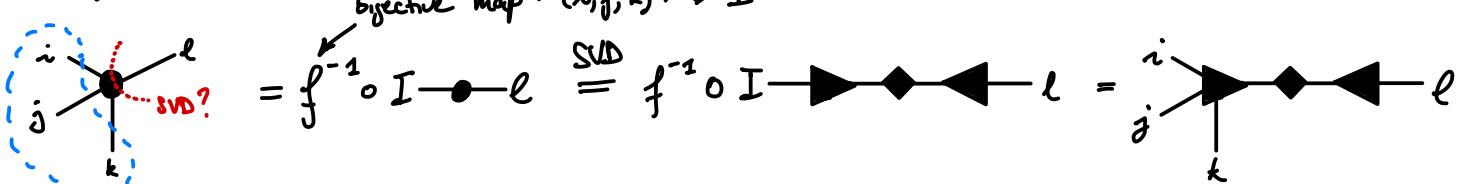
- M normal ($M = AA^*$) $\xrightarrow[\text{spectral theorem}]{\Rightarrow} M = U D U^+$ with unitary U & diagonal D . If $M \geq 0$, then $D \geq 0$ and $D = \Lambda$.

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?

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

$$\stackrel{\text{SVD}}{=} f^{-1} \circ i_1 \rightarrow \boxed{} \rightarrow \boxed{} \rightarrow I = i_1 \rightarrow \boxed{} \rightarrow \dots \rightarrow \boxed{}_{i_2} \rightarrow \dots \rightarrow \boxed{}_{i_{L-1}} \rightarrow I = \tilde{f}^{-1} \circ I \rightarrow i_L$$

$$\stackrel{\text{SVD}}{=} \tilde{f}^{-1} \circ \overset{\approx}{I} \rightarrow \boxed{} \rightarrow \boxed{} \rightarrow i_L = i_1 \rightarrow \boxed{}_{i_2} \rightarrow \dots \rightarrow \boxed{}_{i_{L-1}} \rightarrow i_L = \tilde{f}^{-1} \circ i_2 \rightarrow \overset{\approx}{I}$$

$$\stackrel{\text{SVD}}{=} \tilde{f}^{-1} \circ i_2 \rightarrow \boxed{} \rightarrow \boxed{} \rightarrow \overset{\approx}{I} = i_1 \rightarrow \boxed{}_{i_2} \rightarrow \dots \rightarrow \boxed{}_{i_{L-1}} \rightarrow i_L$$

⋮ repeat

$$= \begin{array}{ccccccccc} \rightarrow & \rightarrow & \rightarrow & \rightarrow & \dots & \rightarrow & \rightarrow & \dots & \rightarrow & \rightarrow \\ i_1 & i_2 & i_3 & i_4 & & i_l & i_{l+1} & i_{L-3} & i_{L-2} & i_L \end{array} \quad \begin{array}{c} \nearrow \text{red arrow} \\ U^{[i_2]} \end{array} \quad \begin{array}{c} \nearrow \text{red arrow} \\ A(l) = \begin{pmatrix} s_1 & \theta \\ 0 & s_{L-l} \end{pmatrix} \end{array} \quad \begin{array}{c} \nearrow \text{red arrow} \\ V^{[i_{L-2}]} \end{array}$$

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

Why scalar?

→ $U^{[i_2]}, V^{[i_L]}$ are vectors

for fixed i_2, i_L

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

Reduced density matrix

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

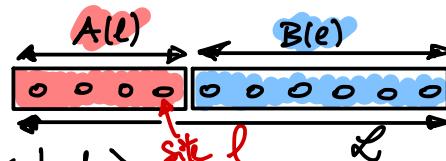
$$\hat{\rho}_A = \text{tr}_B \hat{\rho} = \sum_{\{\phi_B\}} \langle \phi_B | \Psi \rangle \langle \Psi | \phi_B \rangle$$

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

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)

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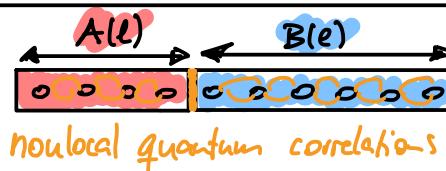
$$= S_m(\tilde{l}) S_{m'}^*(\tilde{l}) U_{mj} U_{m'j'}^* \underbrace{\langle \phi_{B,n} | \phi_{B,j} \rangle}_{\delta_{nj}} \underbrace{\chi \langle \phi_{B,j'} | \phi_{B,n'} \rangle}_{\delta_{n'j'}} |\psi_{A,m} \rangle \langle \psi_{A,m'}|$$

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

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

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

Entanglement entropies



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

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

↳ 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)

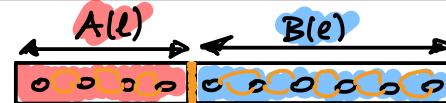
$$S_\alpha(l) = \frac{1}{\alpha-1} \ln \text{tr} \hat{\rho}_A^\alpha$$

Gives entropy from microstates distribution

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

microstate probability

Entanglement entropies



nonlocal quantum correlations

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

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

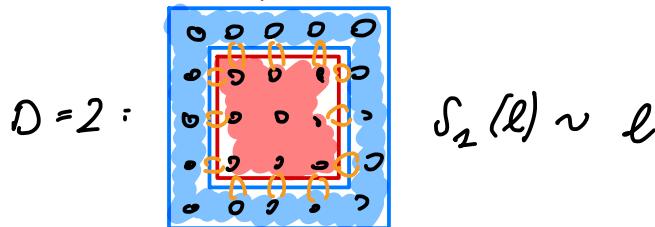
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$$S_\alpha(l) = \frac{1}{\alpha-1} \ln \text{tr} \hat{\rho}_A^\alpha$$

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



$D=1$ 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

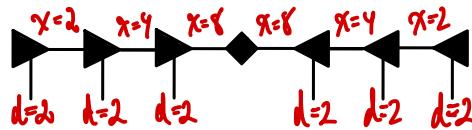
$$S_1 = -\text{tr} \Lambda^2 \ln \Lambda^2$$

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

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}

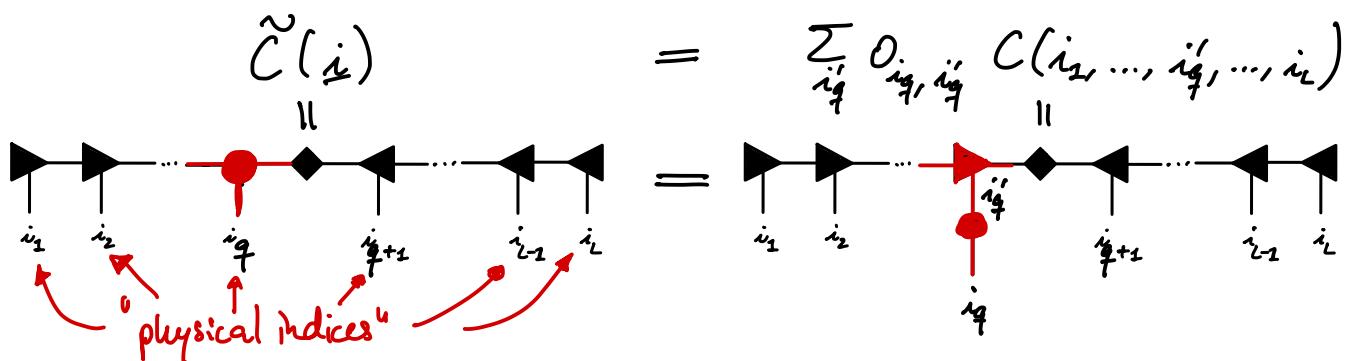
$$\tilde{C}(i) = \sum_{i_1} O_{i_1, i_2} C(i_1, \dots, i'_q, \dots, i_l)$$

3) Matrix Product Operators (MPO)

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

Action on generic MPS:

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



⇒ 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 $L=3$:

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

$$H_2 = \boxed{h_2^2 + jx_1x_2 + h_2}, \quad H_3 = \boxed{h_2^2 + jx_2x_3 + h_2^2 + jx_1x_2 + h_2^2}$$

$$\Rightarrow \prod_{i=1}^L \hat{W}_i = \begin{pmatrix} \hat{I}_L & \hat{\sigma}_L & \hat{H}_L \\ 0 & 0 & \hat{J}\hat{\sigma}_2 \\ 0 & 0 & \hat{I}_L \end{pmatrix} \Rightarrow \hat{H} = (1 \ 0 \ 0) \begin{pmatrix} \hat{I}_L & \hat{\sigma}_L & \hat{H}_L \\ 0 & 0 & \hat{J}\hat{\sigma}_2 \\ 0 & 0 & \hat{I}_L \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = (1 \ \hat{\sigma}_L \ \hat{H}_L) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hat{H}_L \quad \checkmark$$

Graphical notation

$$\hat{W}_q = \left\{ \left(W_q^{lm} \right)_{i\bar{q}, i\bar{q}} \mid i\bar{q} \chi_{i\bar{q}} \right\}_{l,m} = \left\{ \begin{matrix} & i\bar{q} \\ l & \bullet \\ & i\bar{q} \end{matrix} \mid m \right\}_{l,m}$$

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

Energy expectation value

$$\langle \Psi | \hat{H} | \Psi \rangle = \text{Diagram showing a circuit with two horizontal layers of three qubits each. The top layer consists of three diamond-shaped nodes connected by a horizontal line. The bottom layer consists of three circle-shaped nodes connected by a horizontal line. Between the two layers are six triangle-shaped nodes, one between each pair of nodes in the same position. Ellipses indicate that this pattern repeats for more qubits. To the right of the circuit, there are two curly braces: one above the top layer labeled } \hat{C}(\underline{i}) \text{ and one below the bottom layer labeled } \hat{C}^*(\underline{i}').$$

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:

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

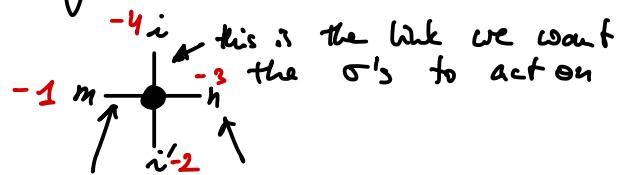
This can be implemented efficiently and then passed to a sparse eigenvalue solver (e.g. ARPACK-package).

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

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

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

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

Check your construction for small system size

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

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

$$LWWWWWR = \dots$$