MPS.1 Reshaping generic tensor into MPS form

A generic tensor of arbitrary rank can be expressed as an MPS through repeated matrix factorizations, using QR decomposition, $M \overset{\text{TNB-III.2}}{=} QR$, or singular value decomposition (SVD): $M \overset{\text{TNB-III.2}}{=} USV^\dagger$

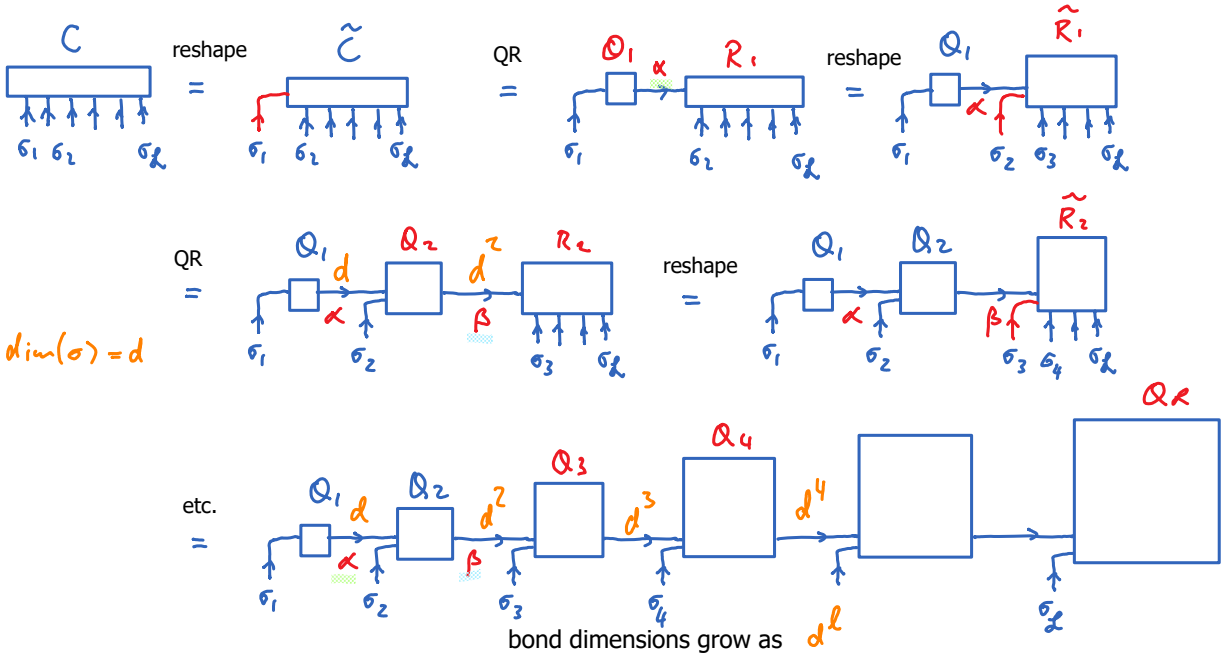
$M^a_b = Q^a_c R^c_b$ $\qquad$ $M^a_b = U^a_c S^c_d V^\dagger{}^d_e$

$$C^{\sigma_1 \dots \sigma_\ell} \overset{\text{reshape (= regroup indices)}}{=} \tilde{C}^{\sigma_1, \sigma_2 \dots \sigma_\ell} \overset{\text{QR}}{=} Q_1^{\sigma_1}{}_\alpha \, R_1^{\alpha, \sigma_2 \dots \sigma_\ell} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_\alpha \, \tilde{R}_1^{\alpha \sigma_2, \sigma_3 \dots \sigma_\ell} \quad (1)$$

$$\overset{\text{QR}}{=} Q_1^{\sigma_1}{}_\alpha \, Q_2^{\alpha \sigma_2}{}_\beta \, R_2^{\beta, \sigma_3 \dots \ell} \overset{\text{reshape}}{=} Q_1^{\sigma_1}{}_\alpha \, Q_2^{\alpha \sigma_2}{}_\beta \, \tilde{R}_2^{\beta \sigma_3, \sigma_4 \dots \ell} \overset{\text{etc.}}{=} \dots \quad (2)$$

$$= Q_1^{\sigma_1}{}_\alpha \, Q_2^{\alpha \sigma_2}{}_\beta \, Q_3^{\beta \sigma_3}{}_\gamma \dots Q_\ell^{\mu \sigma_\ell} \quad (3)$$

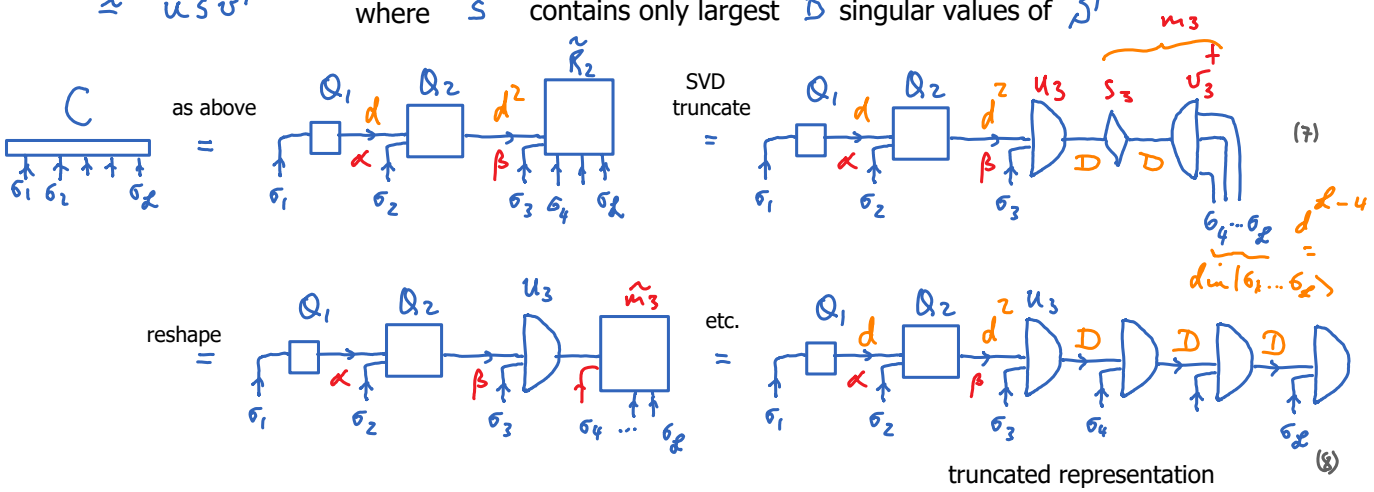
Visualization:



If a maximal bond dimension of $D_\alpha < D$ is desired, this can be achieved using SVD instead of QR decompositions, and truncating by retaining only largest D singular values at each step:

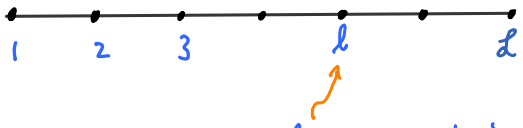
$R \overset{\text{SVD}}{=} USV^\dagger$ (U and V are isometries, S is diagonal, with non-negative elements)

truncate $\simeq USV^\dagger$ where S contains only largest D singular values of S



MPS.1 Iterative diagonalization [generates an MPS]

Consider a spin-s chain, with Hamiltonian $H^{\mathcal{L}} = J \sum_{l=1}^{\mathcal{L}-1} \vec{S}_l \cdot \vec{S}_{l+1} + \sum_{l=1}^{\mathcal{L}} \vec{S}_l \cdot \vec{h}_l$ (1)



local state space for site l : $|\sigma_l\rangle$, $\sigma_l = 1, \dots, d = 2s+1$

We seek eigenstates of $H^{\mathcal{L}}$: $H^{\mathcal{L}} |E_\alpha^{\mathcal{L}}\rangle = E_\alpha^{\mathcal{L}} |E_\alpha^{\mathcal{L}}\rangle$, $|E_\alpha^{\mathcal{L}}\rangle \in \mathcal{H}^{\mathcal{L}}$ (2)

$\alpha = 1, \dots, d^{\mathcal{L}}$

Diagonalize Hamiltonian iteratively, adding one site at a time:

$\mathcal{L}$ =1: Start with first site, diagonalize H^1 in Hilbert space $\mathcal{H}^1$. Eigenstates have form

$$|\alpha\rangle \equiv |E_\alpha^1\rangle = |\sigma_1\rangle A^{\sigma_1}{}_\alpha \qquad (\alpha = 1, \dots, d)$$ (3)

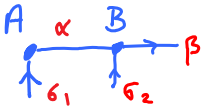
(sum over σ_1 implied) coefficient matrix combine 'incoming' σ_1 into 'outgoing' α

$\mathcal{L}$ =2: Add second site, diagonalize H^2 in Hilbert space $\mathcal{H}^2$:

$$|\beta\rangle \equiv |E_\beta^2\rangle = |\alpha\rangle \otimes |\sigma_2\rangle B^{\alpha\sigma_2}{}_\beta \qquad (\beta = 1, \dots, d^2)$$ (4)

(sum over α, σ_2 implied) coefficient tensor combine 'incoming' α, σ_2 into 'outgoing' β

$$= \underbrace{|\sigma_1\rangle \otimes |\sigma_2\rangle}_{|\vec{\sigma}\rangle_2} A^{\sigma_1}{}_\alpha B^{\alpha\sigma_2}{}_\beta$$

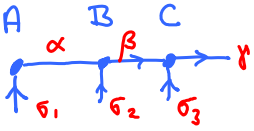


'matrix multiplication' for 'contracted' index α

$\mathcal{L}$ =3: Add third site, diagonalize H^3 in Hilbert space $\mathcal{H}^3$:

$$|\gamma\rangle = |\beta\rangle \otimes |\sigma_3\rangle C^{\beta\sigma_3}{}_\gamma \qquad (\gamma = 1, \dots, d^3)$$ (5)

$$= \underbrace{|\sigma_1\rangle \otimes |\sigma_2\rangle \otimes |\sigma_3\rangle}_{|\vec{\sigma}\rangle_3} A^{\sigma_1}{}_\alpha B^{\alpha\sigma_2}{}_\beta C^{\beta\sigma_3}{}_\gamma$$



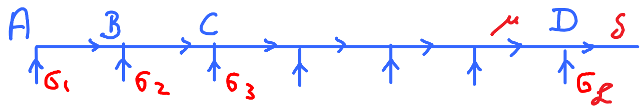
contracted indices α, β

Continue similarly until having added site $\mathcal{L}$. Eigenstates of $H^{\mathcal{L}}$ in $\mathcal{H}^{\mathcal{L}}$ have following structure:

$$|E^{\ell}_{\delta}\rangle = |\delta\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes |\sigma_3\rangle \otimes \ldots \otimes |\sigma_\ell\rangle \underbrace{A^{\sigma_1}{}_{\alpha} B^{\alpha\sigma_2}{}_{\beta} C^{\beta\sigma_3}{}_{\gamma} \ldots D^{\mu\sigma_\ell}{}_{\delta}}_{:= C^{\vec\sigma}{}_{\delta}}$$

$$= |\vec\sigma\rangle_\ell C^{\vec\sigma}{}_{\delta}$$ 'matrix product state' (MPS)

$(\delta = 1, \ldots, d^{\ell})$



Nomenclature: σ_ℓ = physical indices, $\alpha, \beta, \gamma, \ldots$ = (virtual) bond indices

Alternative, widely-used notation: 'reshape' the coefficient tensors, such that physical indices are all upstairs (high), others all downstairs (low):

$$\tilde{A}^{\sigma_1}_{\alpha} := A^{\sigma_1}{}_{\alpha}, \quad \tilde{B}^{\sigma_2}_{\alpha\beta} := B^{\alpha\sigma_2}{}_{\beta}, \quad \tilde{C}^{\sigma_3}_{\beta\gamma} := C^{\beta\sigma_3}{}_{\gamma}$$

to highlight 'matrix product' structure in noncovariant notation:

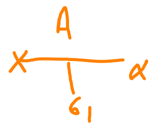
$$|\delta\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes |\sigma_3\rangle \otimes \ldots \otimes |\sigma_\ell\rangle \tilde{A}^{\sigma_1}_{\alpha} \tilde{B}^{\sigma_2}_{\alpha\beta} \tilde{C}^{\sigma_3}_{\beta\gamma} \ldots \tilde{D}^{\sigma_\ell}_{\mu\delta}$$

Comments

1. Iterative diagonalization of 1D chain generates eigenstates whose wave functions are tensors that are expressed as matrix products.

Such states an called 'matrix product states' (MPS)

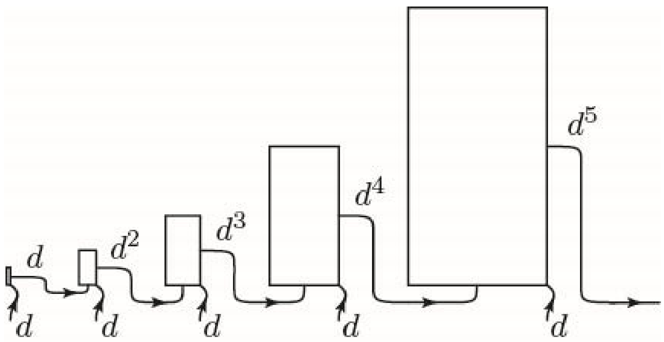
Matrix size grows exponentially:



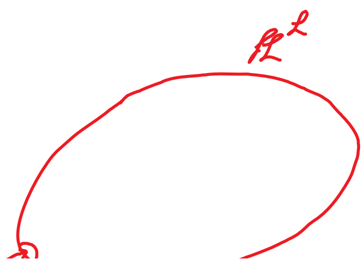
for given σ_1, $A^{\sigma_1}_{\alpha_0\,\alpha}$ has dimension $1 \times d$ (vector)

for given σ_2, $B^{\alpha\sigma_2}{}_{\beta}$ has dimension $d \times d^2$ (rectangular matrix)

for given σ_3, $C^{\beta\sigma_3}{}_{\gamma}$ has dimension $d^2 \times d^3$ (larger rectangular matrix)



$\ldots \quad d^{\ell}$



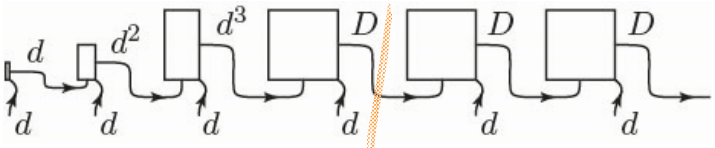
'Hilbert space is a large place'

'Hilbert space is a large place'

Numerical costs increase exponentially with increasing L, so truncation schemes will be needed...

Truncation can be done in controlled way using tensor network methods!

Standard truncation scheme: use $\alpha, \beta, \gamma, \ldots \leq D$ for all virtual bonds



$S_{LR} \leq \ln D$

2. Number of parameters available to encode state:

$N_{MPS} \leq L D^2 d$

would be '=' if all virtual bonds have the same dimension, D :

D, $\ln D$, $\sim d$

$A^{\mu} \sigma_{\lambda} \sim D$

N_{MPS} scales linearly with system size,

If L is large: $N_{MPS} \ll d^L$

Why should this have any chance of working? Remarkable fact: for 1d Hamiltonians with local interactions and a gapped spectrum, ground state can be accurately represented by MPS!

Why? 'Area laws'! (TNB-1.2)

Periodic Boundary conditions

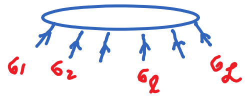
MPS.2 Overlaps, matrix elements

MPS.2

Overlaps $\langle\tilde\psi|\psi\rangle$

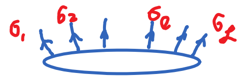
We first consider general quantum states, then matrix product states (MPSs):

General ket: $|\psi\rangle = |\sigma_1\rangle|\sigma_2\rangle \dots |\sigma_\mathscr{L}\rangle C^{\sigma_1 \dots \sigma_\mathscr{L}} =: |\vec\sigma\rangle C^{\vec\sigma}$ $\quad (\in \mathcal{H}^{\mathscr{L}})$ (1)



summation over repeated indices implied

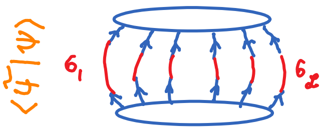
General bra: $\langle\psi| = \overline{C^{\sigma_1,\dots,\sigma_\mathscr{L}}}\, \langle\sigma_\mathscr{L}|\dots\langle\sigma_2|\langle\sigma_1| =: C^\dagger_{\vec\sigma_R}\langle\vec\sigma|$, with $\overline{C^{\sigma_1,\dots,\sigma_\mathscr{L}}} := C^\dagger_{\vec\sigma_R}$, $C^\dagger_{\vec\sigma_R} = \overline{C^{\vec\sigma}}$ (2)



Overlap: $\langle\tilde\psi|\psi\rangle = \overline{\tilde C^{\sigma'_1,\dots,\sigma'_\mathscr{L}}}\,\langle\sigma'_\mathscr{L}|\dots\langle\sigma'_2|\langle\sigma'_1|\sigma_1\rangle|\sigma_2\rangle\dots|\sigma_\mathscr{L}\rangle C^{\sigma_1,\dots,\sigma_\mathscr{L}}$ (3a)

These unit matrices lead to contractions, depicted graphically by connected legs! $\rightsquigarrow \mathbb{1}^{\sigma'_\mathscr{L}}{}_{\sigma_\mathscr{L}}\dots\mathbb{1}^{\sigma'_2}{}_{\sigma_2}\,\mathbb{1}^{\sigma'_1}{}_{\sigma_1} = \mathbb{1}^{\vec\sigma'}{}_{\vec\sigma}$

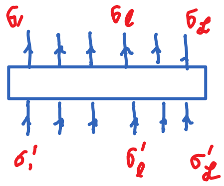
$$= \tilde C^\dagger_{\vec\sigma}\, C^{\vec\sigma}$$



(3b)

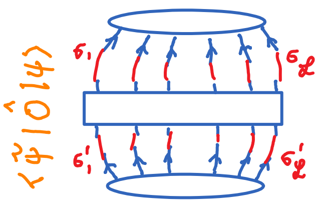
Recipe for overlaps: contract all physical legs of bra and ket.

General operator: $\hat O = |\vec\sigma'\rangle O^{\vec\sigma'}{}_{\vec\sigma}\langle\vec\sigma|$ (4)



Matrix elements: $\langle\tilde\psi|\hat O|\psi\rangle = C^\dagger_{\tilde{\vec\sigma}_R}\langle\tilde{\vec\sigma}|\vec\sigma'\rangle O^{\vec\sigma'}{}_{\vec\sigma}\langle\vec\sigma|\tilde{\vec\sigma}\rangle C^{\tilde{\vec\sigma}}$, with $\langle\tilde{\vec\sigma}|\vec\sigma'\rangle = \mathbb{1}^{\tilde{\vec\sigma}'}{}_{\vec\sigma'}$, $\langle\vec\sigma|\tilde{\vec\sigma}\rangle = \mathbb{1}^{\vec\sigma}{}_{\tilde{\vec\sigma}}$ (5a)

$$= C^\dagger_{\vec\sigma'_R}\, O^{\vec\sigma'}{}_{\vec\sigma}\, C^{\vec\sigma}$$



(5b)

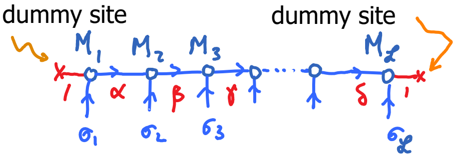
Recipe for matrix elements: contract all physical legs of bra and ket with operator.

Now consider matrix product states:

Ket: dummy index

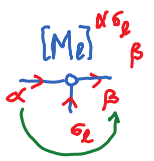
$|\psi\rangle = |\vec\sigma\rangle [M_1]^{1\sigma_1}{}_\alpha [M_2]^{\alpha\sigma_2}{}_\beta [M_3]^{\beta\sigma_3}{}_\gamma \dots [M_\mathscr{L}]^{\gamma\sigma_\mathscr{L}}{}_1$

dummy index



(6)

Recipe for ket formula: as chain grows, attach new matrices M_ℓ on the right (in same order as vertices in diagram), resulting in a matrix product of M^σ matrices .



The subscript ℓ on M_ℓ indicates that the tensors differ from site to site. The tensor M_ℓ has elements $[M_\ell]^{\alpha\sigma_\ell}{}_\beta$, indicated using square brackets.

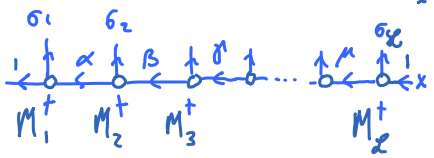
Add dummy sites at left and right, so that first and last M's have two virtual indices, just like other M's .

Bra:

index-reading order

$$\langle\psi| = \overline{[M_1]}^{\sigma_1}_{\alpha}\,\overline{[M_2]}^{\alpha\sigma_2}_{\beta}\,\overline{[M_3]}^{\beta\sigma_3}_{\gamma}\cdots\overline{[M_\ell]}^{\gamma\sigma_\ell}_{1}\,\langle\vec{\sigma}| \qquad \overline{M^{\sigma}}_{\alpha\beta} =: M^{\dagger}{}^{\alpha\sigma}_{\beta} \qquad (7a)$$

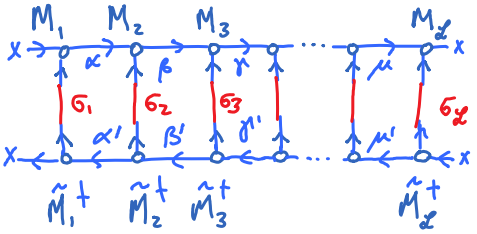
$$= [M_\ell^\dagger]^{\sigma_\ell\mu}\cdots[M_3^\dagger]^{\gamma\sigma_3}[M_2^\dagger]^{\beta\sigma_2\alpha}[M_1^\dagger]^{\alpha\sigma_1}\,\langle\vec{\sigma}| \qquad (7b)$$



We expressed all matrices via their Hermitian conjugates by transposing indices and inverting arrows.
To recover a matrix product structure, we ordered the Hermitian conjugate matrices to appear in the opposite order as the vertices in the diagram.

Recipe for bra formula: as chain grows, attach new matrices $M^\dagger_\sigma$ on the left,
(in opposite order as vertices in diagram), resulting in a matrix product of $M^\dagger_\sigma$ matrices.

Overlap: $\langle\tilde{\psi}|\psi\rangle \overset{(3b)}{=}$



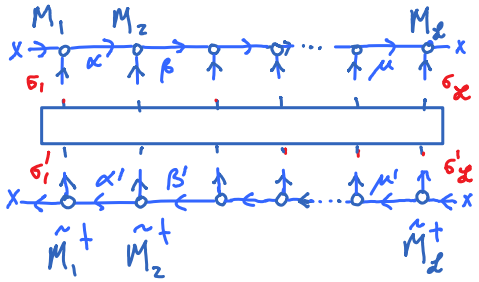
Recipe: contract all physical indices! (8a)

$$= [\tilde{M}_\ell^\dagger]^{\sigma_\ell\mu'}\cdots[\tilde{M}_2^\dagger]^{\beta'\sigma_2\alpha'}[\tilde{M}_1^\dagger]^{\alpha'\sigma_1}[M_1]^{\sigma_1}\,\alpha\,[M_2]^{\alpha\sigma_2}\,\beta\cdots[M_\ell]^{\mu\sigma_\ell} \qquad (8b)$$

Recipe: contract all physical indices with each other, and all virtual indices of neighboring tensors.

Matrix elements

$$\langle\tilde{\psi}|\hat{O}|\psi\rangle \overset{(5b)}{=}$$



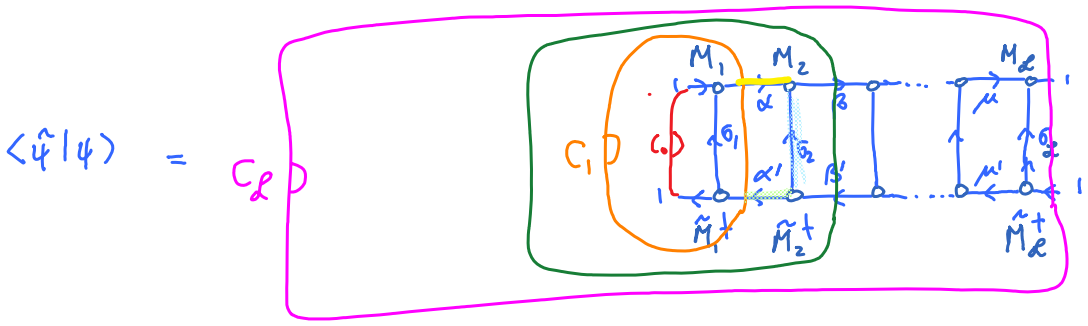
(9)

$$= [\tilde{M}_\ell^\dagger]^{\sigma'_\ell\mu'}\cdots[\tilde{M}_2^\dagger]^{\beta'\sigma'_2\alpha'}[\tilde{M}_1^\dagger]^{\alpha'\sigma'_1}\,O^{\sigma'_1\sigma'_2\ldots\sigma'_\ell}_{\sigma_1\sigma_2\ldots\sigma_\ell}\,[M_1]^{\sigma_1}\,\alpha\,[M_2]^{\alpha\sigma_2}\,\beta\cdots[M_\ell]^{\mu\sigma_\ell} \qquad (10)$$

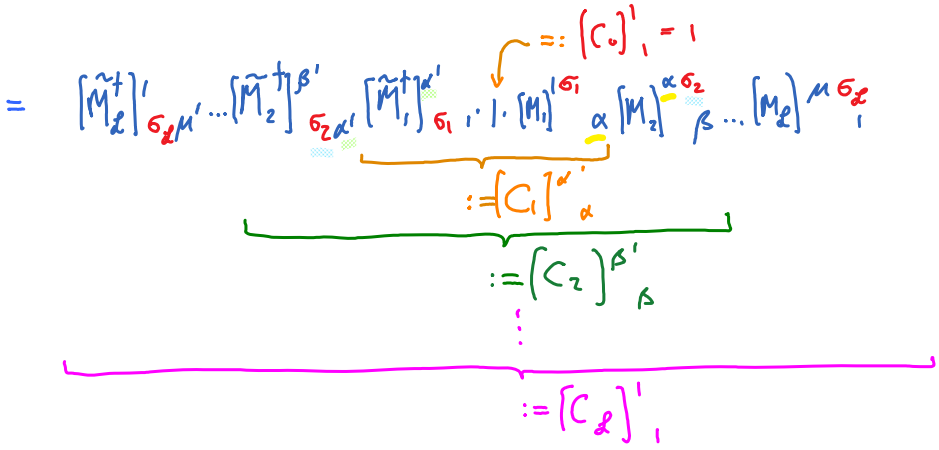
Exercise: derive this result algebraically from (7a), (8a)!

If we would perform the matrix multiplication first, for fixed $\vec{\sigma}$, and then sum over $\vec{\sigma}$,
we would get d^ℓ terms, each of which is a product of 2ℓ matrices. Exponentially costly! ☹

But calculation becomes tractable if we rearrange summations, to keep number of 'open legs' as small as possible (here = 2):

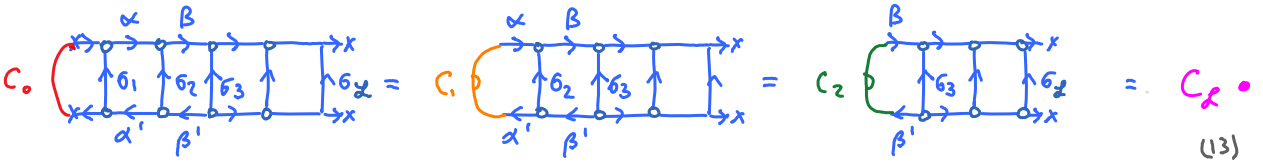


(11)



(12)

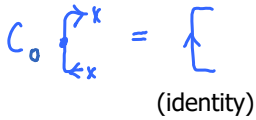
Diagrammatic depiction: 'closing zipper' from left to right.



(13)

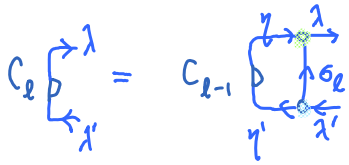
The set of two-leg tensors C_ℓ can be computed iteratively:

Initialization:



$C^1_{[0]\,1} = 1$ (14)

Iteration step:
sum over σ_ℓ
yields C_ℓ



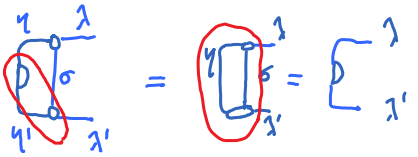
$[C_\ell]^{\lambda'}{}_{\lambda} = [\tilde{M}_\ell^\dagger]^{\lambda'}{}_{\sigma_\ell\,\eta'} [C_{\ell-1}]^{\eta'}{}_{\eta} [M_\ell]^{\eta\sigma_\ell}{}_{\lambda}$ (15)

Final answer: $\langle\tilde{\psi}|\psi\rangle = [C_\ell]^1{}_1$ (16)

Cost estimate (if all A's are $D \times D$):

One iteration:

$D^2 d$	D	D^2	Dd
fixed	sum	fixed	sum
$\lambda'\eta\sigma$	η'	$\lambda'\lambda$	$\eta\sigma$

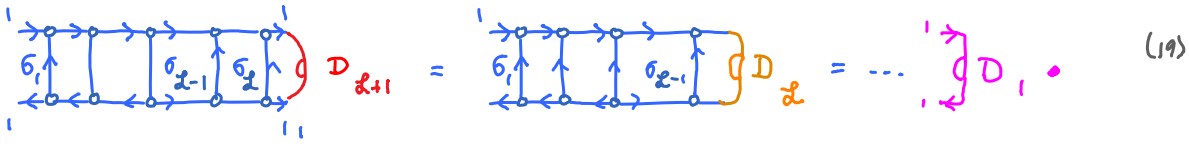


(17)

fixed sum fixed sum

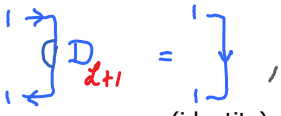
Total cost: $\sim D^3 d \cdot \ell$ (18)

Remark: a similar iteration scheme can be used to 'close zipper from right to left':



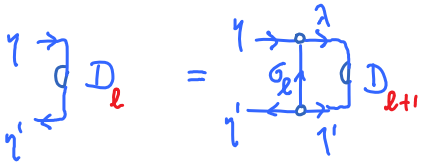
(19)

Initialization:



(identity)

iteration step: sum over σ_ℓ yields D_ℓ



(20)

Normalization $\langle \psi | \psi \rangle = ?$ Use above scheme, with $\tilde{M} = M$

'Closing the zipper' is also useful for computing expectation values of local operators,
i.e. operators acting non-trivially only on a few sites (e.g. only one, or two nearest neighbors).

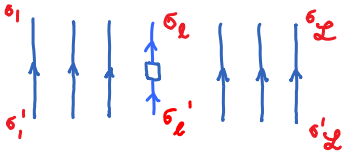
One-site operator (acts non-trivially only on one site, ℓ)

Action on site ℓ : $\hat{O}_\ell = |\sigma_\ell'\rangle [O]^{\sigma_\ell'}_{\sigma_\ell} \langle \sigma_\ell|$

(21)

E.g. for spin ½ : $[S^z]^{\sigma'}_{\sigma} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $[S^+]^{\sigma'}_{\sigma} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $[S^-]^{\sigma'}_{\sigma} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

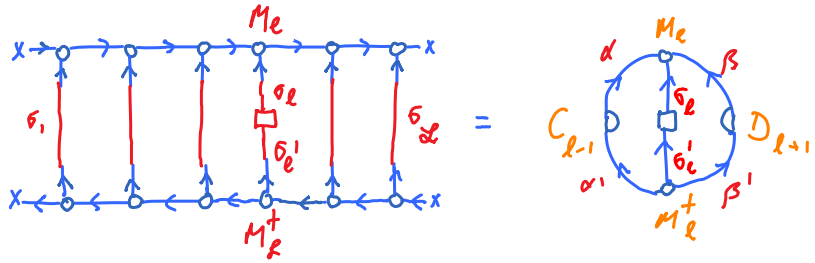
Action on full chain: $\hat{O}_\ell = |\vec{\sigma}'\rangle \mathbb{1}^{\sigma_1'}_{\sigma_1} \cdots [O]^{\sigma_\ell'}_{\sigma_\ell} \cdots \mathbb{1}^{\sigma_L'}_{\sigma_L} \langle \vec{\sigma}|$, $O^{\vec{\sigma}'}_{\vec{\sigma}}$



(22)

Matrix element between two MPS:

$\langle \tilde{\psi} | \hat{O} | \psi \rangle =$



(23)

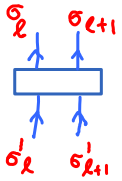
Close zipper from left using $C_{\ell-1}$ [see (15)] and from right using $D_{\ell+1}$ [see (20)].

$$= \left[\tilde{M}_\ell^\dagger\right]_{\beta'\sigma_\ell'\alpha'} \left[C_{\ell-1}\right]^{\alpha'}{}_{\alpha} \left[M_\ell\right]^{\alpha\sigma_\ell\beta} \left[D_{\ell+1}\right]_{\beta}{}^{\beta'} \left[0\right]^{\sigma_\ell'}{}_{\sigma_\ell} \qquad (24)$$

Two-site operator (acts nontrivially only on two sites, ℓ and $\ell+1$) [e.g. for spin chain: $\vec{S}_\ell \cdot \vec{S}_{\ell+1}$]

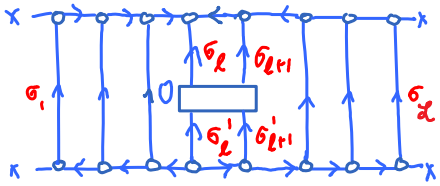
Action on sites ℓ, $\ell+1$:

$$\hat{O}_{\ell,\ell+1} = |\sigma_\ell'\rangle|\sigma_{\ell+1}'\rangle \left[0\right]^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}} \langle\sigma_{\ell+1}|\langle\sigma_\ell| \qquad (10)$$

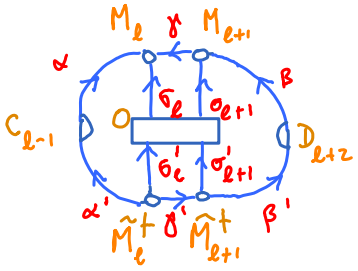


Matrix elements:

$$\langle\tilde{\psi}|\hat{O}_{\ell,\ell+1}|\psi\rangle =$$



$=$



(11)

$$= \left[\tilde{M}_{\ell+1}^\dagger\right]_{\beta'\sigma_{\ell+1}'}{}^{\gamma'} \left[\tilde{M}_\ell^\dagger\right]_{\gamma'\sigma_\ell'\alpha'} \left[C_{\ell-1}\right]^{\alpha'}{}_{\alpha} \left[M_\ell\right]^{\alpha\sigma_\ell\gamma} \left[M_{\ell+1}\right]^{\gamma\sigma_{\ell+1}\beta} \left[D_{\ell+2}\right]_{\beta}{}^{\beta'} \left[0\right]^{\sigma_\ell'\sigma_{\ell+1}'}{}_{\sigma_\ell\sigma_{\ell+1}} \qquad (12)$$